Comparison of Emissions Processing by EM-S95 and SMOKE over the Midwestern U.S.

Allen Williams, Mike Caughey, Ho-Chun Huang, Xin-Zhong Liang, Ken Kunkel
Illinois State Water Survey, 2204 Griffith Dr., Champaign, Il 61820
allenwil@uiuc.edu

Zhining Tao, Susan Larson
Dept. of Civil and Environmental Engineering, University of Illinois, 205 N. Mathews, Urbana, IL 61801

Donald Wuebbles
Dept. of Atmospheric Sciences, University of Illinois, 105 S. Gregory, Urbana, IL 61801

Abstract

The work presented in this paper is part of the development of a climate, air quality, and impact modeling system (CAQIMS) focused on the Midwestern United States. Currently CAQIMS includes a regional climate model (RCM) and an air quality model (AQM). The SMOKE emissions processor uses data from the 1996 National Emissions Trend (NET96) inventory together with meteorological output from the RCM to compute input emissions data for the AQM.

In this paper results from the SMOKE emission processor are compared directly with results from the well-established EMS-95 emission processor. This comparison is done using SMOKE to process an episode emission inventory, provided by the Illinois EPA and the Lake Michigan Air Directors Consortium, that has also been independently processed using EMS-95. In addition, SMOKE output is reported for simulations using the NET96 inventory data over three nested domains from 90 km grid spacing covering the U. S. to 10 km grid spacing over the Midwest for June-August 1995.

The results show that SMOKE and EMS-95 produce emissions with comparable magnitudes. Major differences between the temporalization procedures used by the two processors are identified. Differing temporalization schemes can cause large differences in diurnal emissions patterns, which in turn significantly affect air quality model results. Our comparison demonstrates the need to develop and implement more realistic temporalization schemes.

Introduction

An integrated climate, air quality and impact modeling system (CAQIMS) under development (Kunkel et al., 1999) currently includes a regional climate model (RCM) and an air quality model (AQM). The AQM requires the input of speciated emissions values for each grid square over the entire domain at each model time step. For typical AQM simulations the emissions must be specified at spatial intervals of tens of kilometers and over time intervals of tens of minutes. By contrast, the best available emissions dataset is the 1996 National Emissions Trends (NET96) inventory, where the data are available as annual or seasonal countywide averages. The available data must therefore be processed to produce the input required by the AQM, normally as hourly averaged gridded values. The Emissions Modeling System-95 (EMS-95) has been widely used to process emissions input data. The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (Houyoux et al., 2000) represents a new approach to emissions modeling. Although SMOKE incorporates many of the EMS-95 algorithms to perform the necessary spatial and temporal transformations, it is designed for computational efficiency. The SMOKE processor is being tested for emissions calculation in CAQIMS.

This paper describes preliminary results using SMOKE to process inventory data into temporalized and gridded emissions, ready for input to the AQM. Single-day emissions calculations for June 13th, 1995 are shown where identical inventory data are processed independently using SMOKE and using EMS-95. Emissions are also presented for a 90-day simulation from May 31st through August 28th, 1995, which are being prepared for a CAQIMS baseline simulation.

Description of Emissions Simulations

The 3-way nested domain used for the present study is shown in Figure 1. Domain 1 has a 90-km grid spacing and extends from the Pacific to the Atlantic Oceans, and includes the Gulf of Mexico and much of Canada. This domain is designed with the objective to faithfully transmit the effects of large-scale meteorological features to the Midwest region. This domain configuration produces the most skillful simulation of the observed 1993 summer flood over the Midwest (Liang et al., 2001) and Sep-Oct 1986 heavy precipitation episodes in the central U.S. (Kunkel and Liang, 2001). The RCM realistically simulates both temporal variations and spatial distribution in the major flood area. This success is identified with the accurate representation of both the midlatitude upper-level westerly jet stream, which steers synoptic disturbances into the Midwest, and Great Plains low-level southerly jet, which transports warm, moist and potentially unstable air to the region. Domain 2 extends from just east of the Rocky Mountains to the East Coast, and from the U.S.-Canadian border into the Gulf of Mexico with 30-km grid spacing. Domain 3 covers a section of the Midwest centered on Illinois and Indiana at 10-km grid spacing. These two inner domains are positioned to resolve regional and local meteorological processes, and to accurately simulate air quality over the Midwest.

The CAQIMS baseline simulation focuses on the summer of 1995, during which record heat waves and several ozone episodes occurred. However, the 1996 emissions source inventory is far more complete than any emissions data available for 1995. Annual and ozone season emissions should not change drastically over the period of a year, so the 1996 emission inventory coupled with 1995 meteorology is used for the CAQIMS baseline simulation. Emissions have been processed with SMOKE for the period from May 31st to August 28th for each domain using the NET96 emission inventory as input.

NET96 categorizes emission sources according to a 10-digit source classification code (SCC). Although the SCC numbering system is very specific, emissions are further categorized according to area, mobile, point and biogenic source types due to basic differences in the way they are reported. Point source emissions are specified by the latitude and longitude of a specific exhaust stack with known diameter, height, elevation, temperature and flow rate. By contrast, area emissions are given as averages across entire counties. Mobile emissions are either provided at a county level, similar to area emissions, or, alternatively, as vehicle miles traveled for specific road segments called links. For simplicity, during our initial efforts at running SMOKE, we used county-level mobile emissions data, rather than roadway link data and vehicle miles traveled. We will use link VMT data in future simulations for greater accuracy. For area and point sources, the emissions rates for NO_x, VOC, SO_2, CO etc. are reported both as annual average values and as "ozone season" average values. The point source specification depends on meteorology in that plume rise from stack emissions can lead to source values at elevated levels. For the plume rise calculations meteorological values, in the present case from the RCM, must be input into SMOKE. The NET96 inventory does not contain biogenic data, so countywide VOC and NO_x emissions are calculated. External geographic information system (GIS) land-use data describe the distribution of surface vegetation. The VOC and NO_x emissions are calculated using the surface temperature and other RCM output data.

The level of specificity of the source classification codes used in the NET96 inventory depends largely on the reporting format of the original emissions data. For example, within the area source category, an SCC of 2306010000 represents all emissions from asphalt paving and roofing applications; an SCC of 2401005000 indicates all solvent evaporation from auto refinishing; and 2420000000 indicates all dry cleaning emissions. Similarly for the mobile category an SCC of 2230070000 represents all heavy-duty diesel trucks, while 2230060000 is all light duty diesel trucks. Source classification codes may not only represent the sum of a class, i.e., 2201080000 for all motorcycles, but also more specific subdivisions of that class, such as 2201080110 for all motorcycles on rural interstates, versus 2201080230 for all motorcycles on urban roadways.

The NET96 inventory includes area, mobile and point emissions data. For use by SMOKE the data must be transformed to a column specific ASCII format. SMOKE processing of emissions for use by the CAQIMS is done in script mode. When a grid square includes portions of more than one county, a spatial surrogate file is constructed to apportion county-level area emissions into grid-square-level emissions. The apportionment is done using GIS applications ArcView and ArcInfo. First, the grid for each domain is formed in ArcInfo as a shape file in a Lambert geographic projection. Then ArcView geographically intersects the shape file with a Lambert projection of U.S. counties to determine the area from each constituent county comprising the grid. The countywide mobile emissions from the NET96 data are likewise apportioned into domain grid squares.

In the SMOKE emission processor, the user specifies the time dependence based on source type. Monthly, weekly, diurnal weekday, and diurnal weekend temporal profiles are assigned for each SCC. For example, a simple daily profile for emissions due to space heating might specify lower values from 10:00 PM to 6:00 AM, and higher values from 6:00 AM to 10:00 PM. Similarly, monthly space heating emissions profile would be lowest in the summer, moderate in spring and fall, and highest in the winter.

A simulation for a major ozone episode on July 13, 1995 is also reported. The source inventory and the emissions processed with EMS-95 were provided by Illinois EPA and developed by staff and members of the Lake Michigan Air Directors Consortium (IEPA/LADCO; IEPA, 2000). The IEPA/LADCO source inventory is in EMS-95 format, which can be directly read into SMOKE. The IEPA/LADCO source inventory is an augmented subset of the NET96 inventory. The EMS-95 emissions output data have been very thoroughly prepared for study of ozone episodes, and represent the most complete analysis conducted to date. The EMS-95 results are at a 4-km grid resolution for a domain slightly smaller than Domain 3. The purpose of the comparison with SMOKE processed emissions is to verify that the two emission models are at least in approximate agreement, and to identify areas where the SMOKE simulation needs improvement from the standpoint of specification of spatial surrogates and temporalization schemes.

Results

Accurate temporal concentration profiles for photochemically active emissions are critical from the standpoint of air quality modeling. In the case of ozone formation, for example, precursor emissions that lead to significant concentrations during the brief period of most rapid ozone formation may be very important for determining the ozone concentration. The 24-hour temporal plot in Figure 2 compares the hourly NO_x emissions for the Chicago area, averaged over the Smoke Domain 3 10-km grid output and the EMS-95 4-km grid output. The SMOKE NO_x diurnal variation leads the EMS-95 by approximately 2 hours; this phase difference will have important consequence on the AQM simulation. The total integrated emissions for the two simulations are very close, and the difference is primarily due to the temporalization patterns. In the simulations using SMOKE that are presented here, the temporalization scheme is that included in the SMOKE tutorial, which is focused on states in the Eastern U.S. and may not be optimized for the Midwest.

As an illustration of the temporalization procedure, the several sources shown in Table I comprise 76% of the total area NO_x emissions for Cook County, which includes Chicago. The dominant area emissions sources are aircraft, locomotives, and three classes of off-highway diesel vehicles. The respective temporalization schemes are shown in Figure 3. The off-highway diesel vehicle emissions are higher during working hours, and fall to practically zero during the early morning hours, and to about 1% during the late evening hours. The railroad emissions are at about 6% of the total from 6:00 AM to 6:00 PM and at about 2 % the rest of the time. The aircraft emissions rise from a few percent to 5% at about 6:00 AM and persist at that value until midnight. The main features of the calculated NO_x area emissions shown in Figure 2 for the SMOKE output reflect the imposed temporalization scheme. We will develop more realistic, and thus regional specific, area source emission temporalization procedures that best suit applications in the CAQIMS domain (Fig. 1).

Figure 4 shows that the magnitude of the Chicago NO_x point source emissions, as well as their diurnal temporalization when processed using SMOKE, are comparable to the EMS-95 results. Point sources, such as coal-fired electricity generation plants, are fairly constant and show minor diurnal variation, while various industrial boilers follow a workday pattern. Figure 5 shows the point source NO_x emissions for the St. Louis area. Although the total magnitude of the emissions computed by the two processors is again fairly close, in this case the temporalization is considerably different. Figure 6 shows the variation of the point NO_x emissions in the St Louis area using the two SMOKE temporalization schemes that apply to point sources comprising 80% of the total point NO_x emissions. We will implement more realistic point source emission temporalization schemes for future CAQIMS simulations.

Figures 7A and 7B compare the gridded output area NO_x emissions for both models. The area NO_x emissions results compare well overall; the differences in Figures 7A and 7B are due to the different grid spacing of the two models. The area emissions characteristically show the locations of cities where the area emissions are high. Outside the urban areas, the 4-km grid used with EMS-95 resolves sources that are not visible in the 10-km grid used with SMOKE. A similar comparison of point sources is given by Figures 8A and 8B. Again the outputs of the two models are very similar with the difference attributable to the difference in grid spacing.

Results from the three-month simulation using the SMOKE model and the NET96 source inventory data are shown in Figure 9. The constituent emissions for the three nested domains are equal when integrated over equal areas. The plot shows that the area and point sources are comparable in magnitude for Illinois NO_x emissions and larger than the mobile and biogenic sources. The plotted values are daily averages so the diurnal variation is not present. The diurnal averaging yields a constant mobile source emission. The plots in Figure 9 clearly show the weekly variations, which are imposed by the weekly temporalization schemes for the different sources. The biogenic emissions are driven by meteorology and have peaks that correspond to warmer days. The increase in the curve for area emissions during June is the result of monthly profile specification because of the increase of construction activities.

Conclusions

Comparisons of SMOKE and EMS-95 for the same source data show that the processors produce comparable total emission amounts. However, the model comparison showed considerable differences in the temporalization of the dominant sources. Given the importance of diurnal variation of some emissions we must implement more realistic temporalization according to distinct categories of emission sources. AQM sensitivity studies will help evaluate the benefits of more accurate temporalization schemes. This research effort is currently in progress.

SMOKE results for the 90-day simulation are internally consistent in that the different nested domains give comparable emissions when averaged over the same areas. The geographic distribution of simulated emissions and the relative magnitudes of the point, area, mobile, and biogenic sources appear reasonable. The weekly and monthly temporalizations employed for the 90-day simulation result in observable variations in simulated emissions.

References

Houyoux, Mark R., Jeffrey M. Vukovich, Carlie J. Coats Jr., Neil J. M. Wheeler, and Prasad S. Kasibhatla, 2000: Emission Inventory Development and processing for he Seasonal Model for Regional Air Quality (SMRAQ) project, *J. Geophysical Research,* **105**, 9079-9090.

IEPA, 2000: *Midwest Subregional Modeling: Emission Inventory*. Illinois Environmental Protection Agency Technical Support Document, September 27.

Kunkel, K., J. Angel, M. Caughey, D. Kristovich,, X.-Z. Liang, H. Ochs, A. Williams, Y. Alila, and M. Heidari, 1999: *Illinois State Water Survey Program to Develop an Integrated Climate, Air Quality and Impact Modeling System: A Basis for Achieving Economic, Societal and Environmental Goals in Illinois*. Water Survey Internal Publication, 35 pp. (**available upon request**).

Kunkel, K.E., and X.-Z. Liang, 2001: Regional climate model simulation of a multi-week heavy precipitation episode in the central U.S. *Preprint of Symposium on Precipitation Extremes: Prediction, Impacts, and Responses,* Amer. Meteorol. Soc., Boston, MA, pp. 185-188.

Liang, X.-Z., K.E. Kunkel, and A.N. Samel, 2001: Development of a regional climate model for US Midwest applications. Part 1: Buffer zone treatment. *J. Climate* (**submitted**)

KEYWORDS

Emissions modeling
SMOKE
EMS-95
NET96
CAQIMS
Midwest
Illinois
Air quality model
Regional climate model
Source temporalization
Ozone
Temporalization

Table I. Sources Comprising 76% of NO_x Area Emissions in Cook County, IL

SCC	Percent of Total Area NOx Emissions	Source Description
2270002000	41	Off-highway Diesel Vehicles: Construction and Mining Equipment
2275020000	12	Commercial Aircraft
2285002000	12	Diesel Railroad Equipment
2270003000	6	Off-highway Diesel Vehicles: Industrial Equipment
2270008000	6	Off-highway Diesel Vehicles: Airport Ground Support Equipment

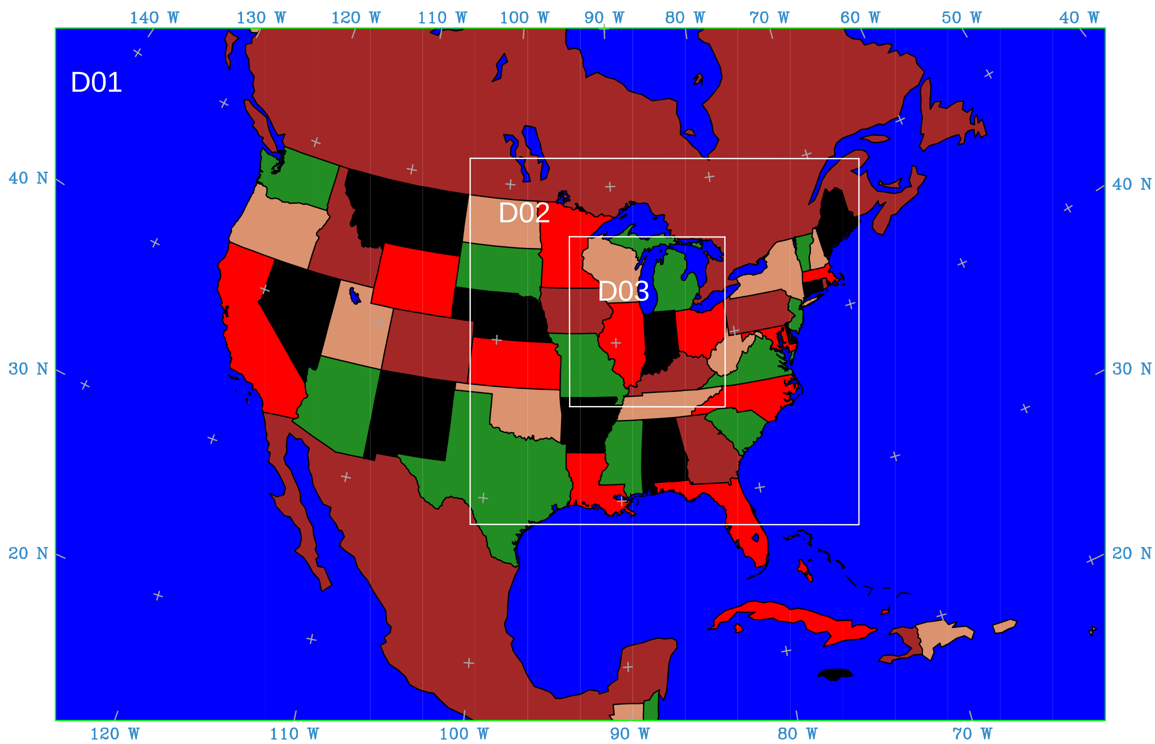

Figure 1. CAQIMS 3-way nested domain with outer domain (D01) at 90 km grid resolution, the intermediate domain (D02) at 30 km resolution, and the inner domain (D03) at 10 km resolution

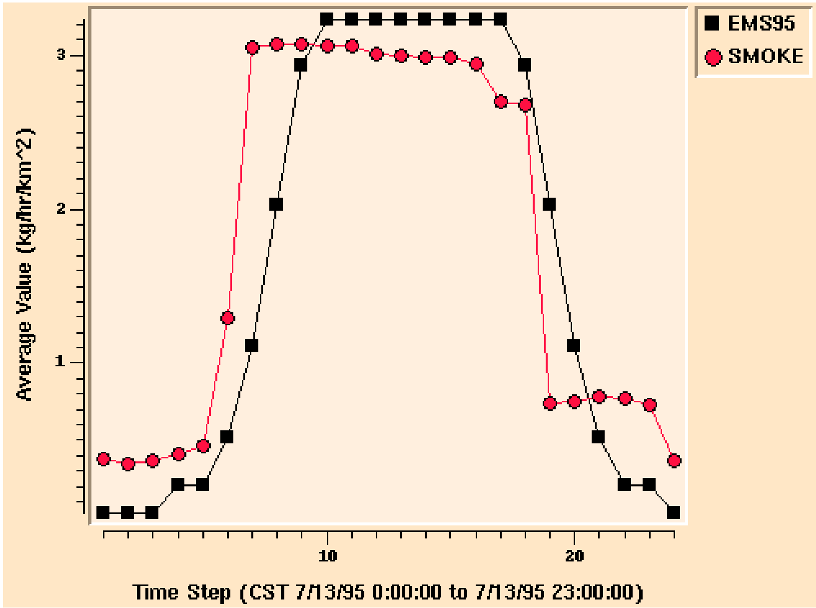

Figure 2. Diurnal area source NO_x emissions in Chicago

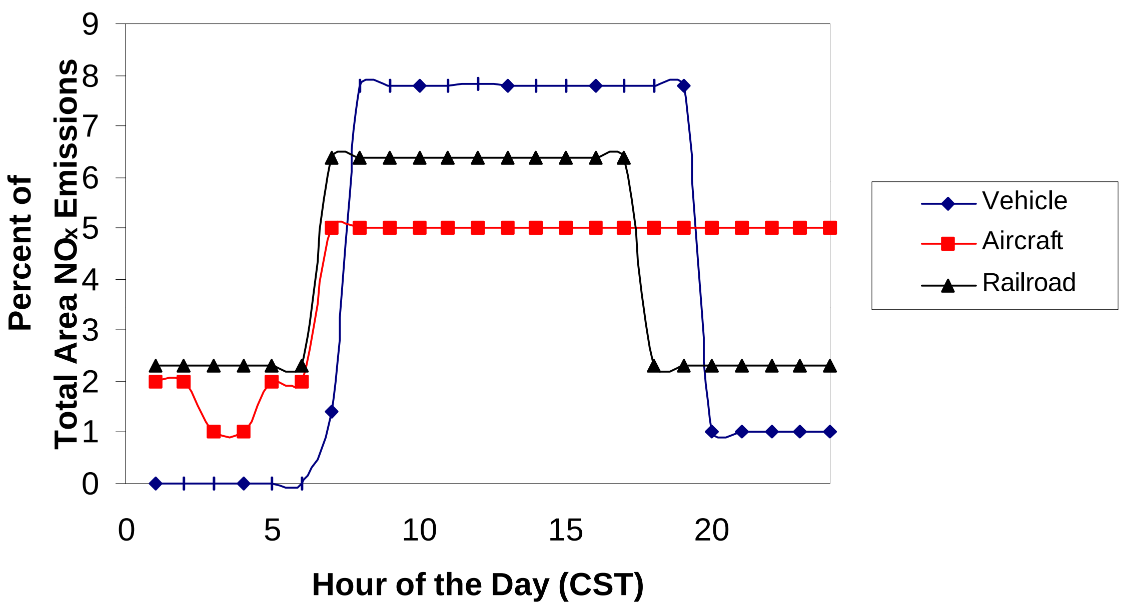

Figure 3. Imposed temporalization patterns for three area source types in Chicago.

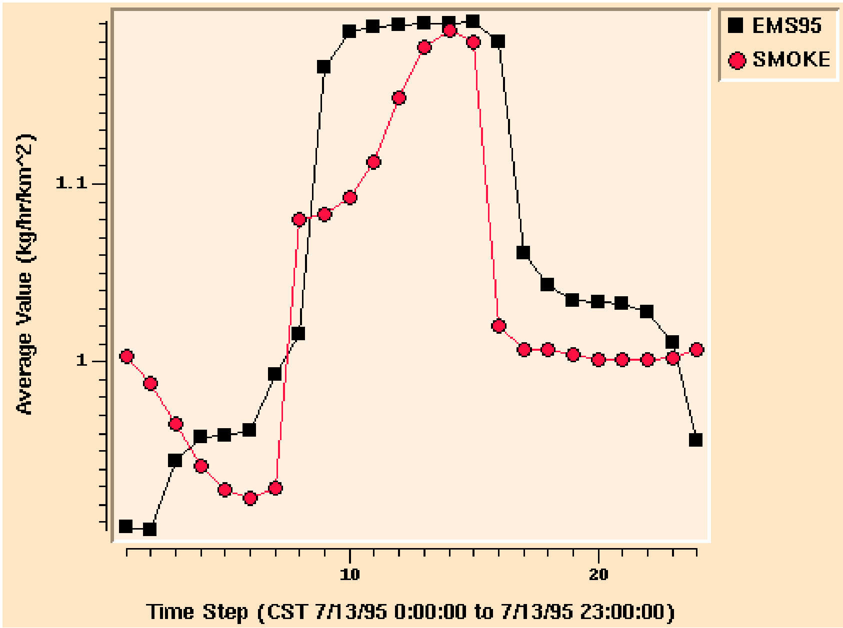

Figure 4. Diurnal point source NO_x emissions in Chicago

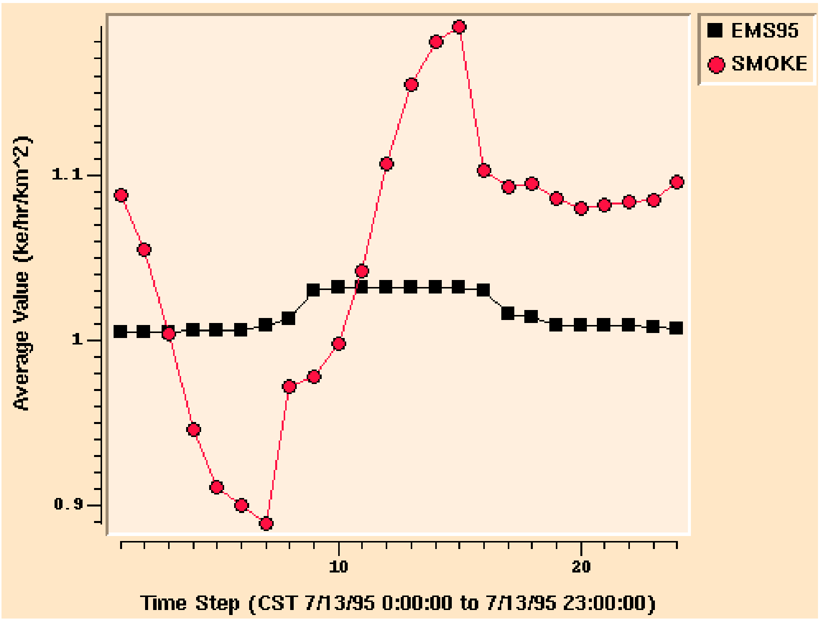

Figure 5. Point source NO_x emissions as a function of time in St. Louis Area.

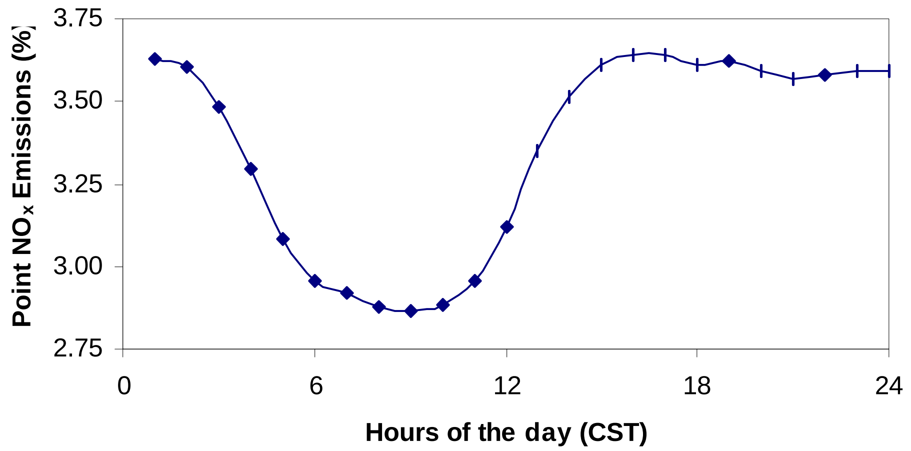

Figure 6. NO_x point emissions (%) in St Louis area using two SMOKE temporalization schemes that account for 80% of mass.

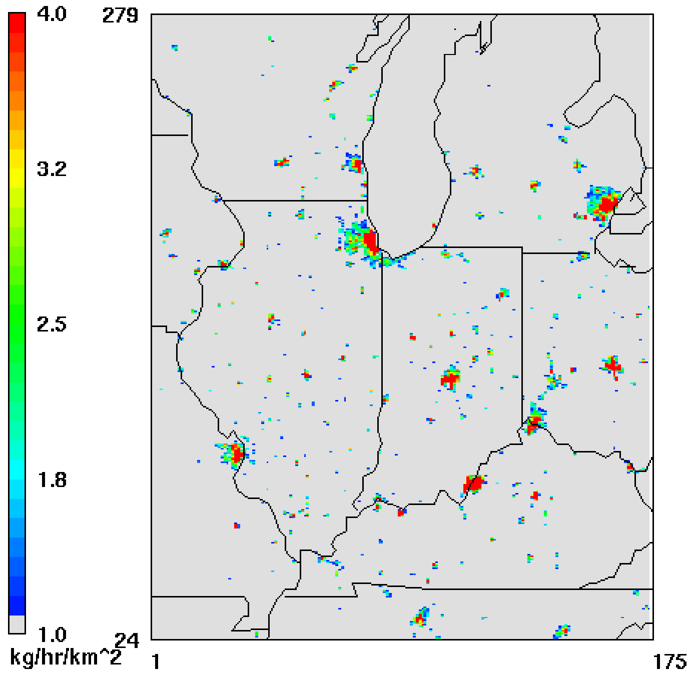

Figure 7A. EMS-95-processed area NO_x emissions (Noon CST 7/13/95)

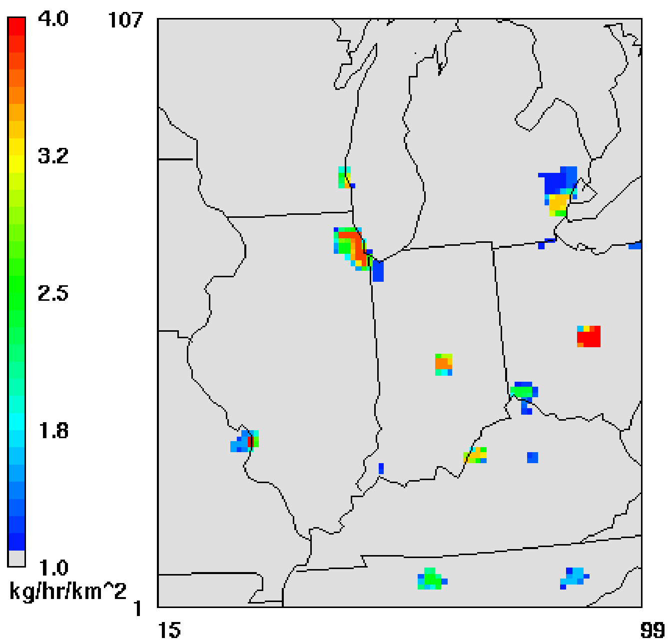

Figure 7B. SMOKE-processed area NO_x emissions (Noon CST 7/13/95)

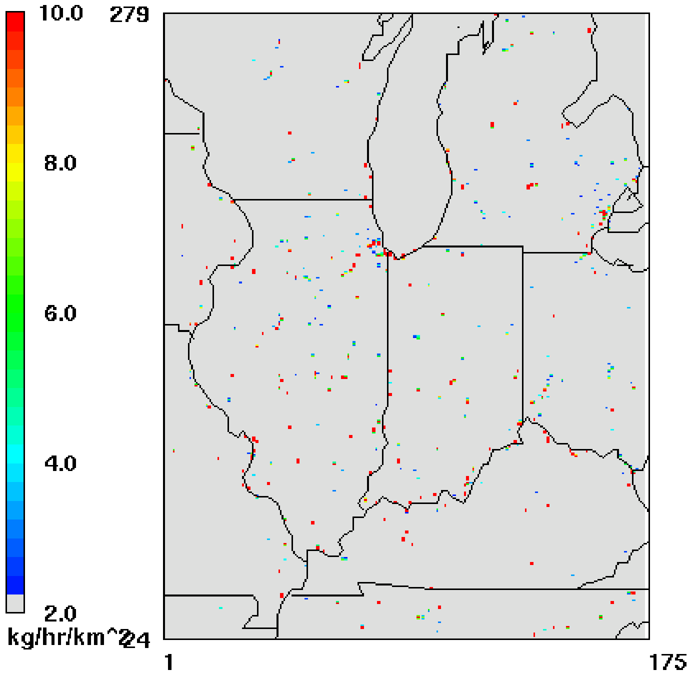

Figure 8A. EMS-95-processed point NO_x emissions (Noon CST 7/13/95)

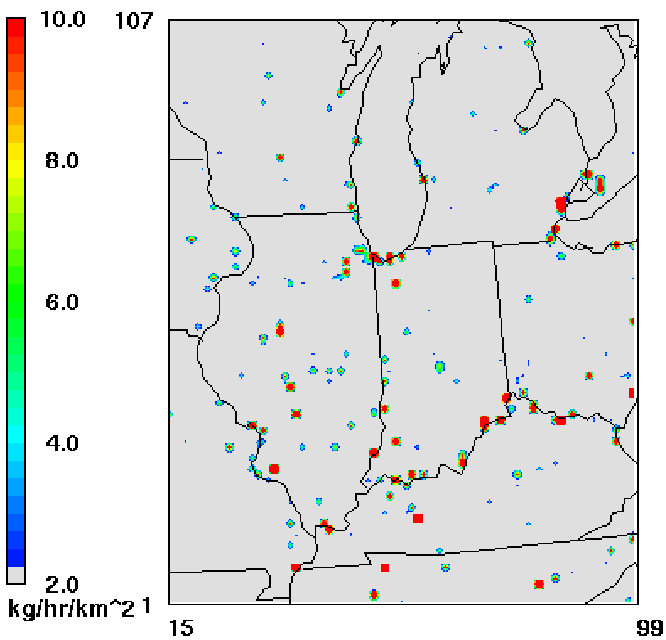

Figure 8B. SMOKE-processed ISWS point NO_x emissions (Noon CST 7/13/95)

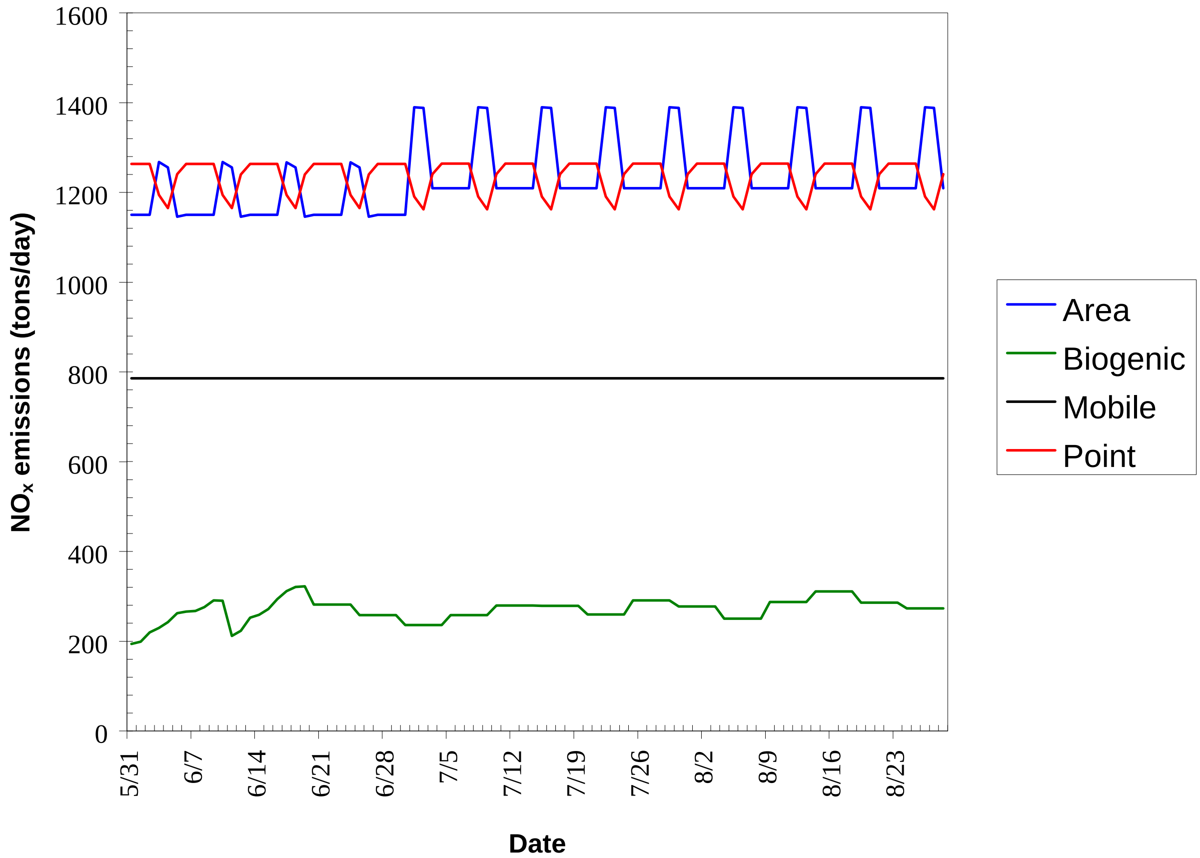

Figure 9. Daily Area NO_x emissions total for all of Illinois