

# **Development of Biogenic Emissions for the 1995 Summer Season Using SMOKE-BEIS2**

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## **ABSTRACT**

Biogenic emissions during the summer of 1995 for the eastern United States have been estimated using the Sparse Matrix Operator Kernel Emissions - Biogenic Emissions Inventory System (SMOKE-BEIS2). Hourly emissions were computed for a modeling grid at a 36 kilometer resolution. The emissions were estimated as part of the Seasonal Model for Regional Air Quality (SMRAQ) effort to model ozone formation and transport from May 15 to September 12, 1995. Estimates were obtained using prognostic meteorology from the Penn State/National Center for Atmospheric Research Mesoscale Modeling System (MM5). Issues concerning the use of prognostic meteorology, other input data and future needs are discussed. The expanded functionality and reporting capabilities of SMOKE-BEIS2 are also described. Additional applications of SMOKE-BEIS2, including an urban-scale grid for North Carolina, have been mentioned to help demonstrate the usefulness of the SMOKE-BEIS2.

## **INTRODUCTION**

The Seasonal Model for Regional Air Quality (SMRAQ) was used to simulate ozone formation and transport for the entire 1995 summer season. This application required gridded emissions estimates be created for the anthropogenic and biogenic sources for the entire season. Estimates of the anthropogenic emissions are discussed in a companion paper.<sup>1</sup> Biogenic emissions of volatile organic compounds (VOCs) and nitric oxide (NO) are important inputs into atmospheric chemistry models and can have a significant effect on the selection of emission control strategies. The Ozone Transport Assessment Group (OTAG) regional modeling study used an emission inventory where over 75% of the VOC emissions came from biogenic sources.<sup>2</sup> The OTAG modeling effort and another study by Pierce and Dudek<sup>3</sup> included generating biogenic emissions estimates for 1995 using observational meteorology. The SMRAQ work incorporated meteorology from a prognostic meteorological model. This paper focuses on the issues we encountered while modeling the gridded biogenic emissions over the entire season.

The background section of this paper summarizes the input data and the modeling system used to calculate the biogenic emissions estimates. The modeling-issues section describes the meteorological and emissions data issues addressed during the SMRAQ application. The results section summarizes the emissions for the summer 1995 season. Finally, the conclusions section summarizes the SMRAQ simulation and discusses the tools needed for simulating biogenic emissions for future seasonal air-quality modeling applications.

## **BACKGROUND**

This section summarizes the input data and modeling system used to produce biogenic emissions for the 1995 summer season. The components include the biogenic emissions modeling system, the modeling domain and episode, the meteorological model used to create input data for the biogenic emissions model, and other data used as input for the biogenic emissions model.

## **SMOKE-BEIS2**

The emissions model used for the SMRAQ project is the Sparse Matrix Operator Kernel Emissions

(SMOKE)<sup>4</sup> modeling system. The biogenic emissions component of the model includes the Urban Airshed Model - Biogenic Emissions Inventory System (UAM-BEIS2)<sup>5</sup> with some modifications. The basic equation used for computing biogenic emissions is given by the following:

$$E = \sum (F_i \times A_i \times M) \quad (1)$$

where  $E$  is the emission rate [gm/hr] for each grid cell,  $F$  is a standardized emission flux [ $\mu\text{g}/\text{m}^2\text{-hr}$ ] for each land use type  $i$ ,  $A$  is the area [ $\text{m}^2$ ] of each land use type  $i$  in a grid cell, and  $M$  is an environmental correction factor that adjusts for the effects of temperature and solar radiation relative to the standard of  $1000 \mu\text{mol}/\text{m}^2\text{-s}$  of visible solar radiation and  $30^\circ\text{C}$  temperature. Biogenic emissions in the model respond quickly to changes in temperature. Isoprene emissions also respond to the amount of solar radiation that reaches the vegetation and are negligible when sunlight is not present. Other documentation outlines the algorithms used to apply the environmental corrections.<sup>6,7</sup> The SMOKE-BEIS2 currently calculates hourly emission rates for species needed for the Carbon Bond IV (CB-IV) mechanism. CB-IV is the chemical mechanism used in the air quality model configuration for the SMRAQ application.<sup>8</sup> The CB-IV species output by SMOKE-BEIS2 are olefins, paraffins, isoprenes, aldehydes, and nitrogen oxide.

The modifications to UAM-BEIS2 made in SMOKE-BEIS2 consist of (1) the correction of an error found in UAM-BEIS2, and (2) conforming to the SMOKE coding standards. The error found dealt with VOC emissions from agricultural land uses not being included in the emissions estimates.

### Modeling Domain and Episode

The episode for the SMRAQ modeling is May 15-September 12, 1995. The horizontal gridded domain (Figure 1) is 72 columns by 74 rows of 36-km-square grid cells using a Lambert projection with a spherical-Earth assumption (to match the meteorological model). The modeling domain includes the eastern half of United States, parts of southern Canada and extreme northeast Mexico. No good data were available for use when creating anthropogenic emissions in Mexico, thus all emissions including biogenic emissions were set to zero in the Mexican grid cells.

### Meteorological Model

The Penn State/National Center for Atmospheric Research Mesoscale Modeling System, version 1 (MM5)<sup>9</sup> provides meteorological input data for SMOKE-BEIS2. MM5 was executed on the same Lambert projection mentioned in the previous section but on a much larger domain containing most of the contiguous United States, southern Canada, and northern Mexico. The Meteorology/Chemistry Interface Processor (MCIP)<sup>8</sup> was used to post-process the MM5 output data for input into SMOKE-BEIS2 and the air quality model. The output from MCIP included two-dimensional gridded data for the net radiation reaching the ground, cloud top and bottom height, cloud cover fraction, and three-dimensional temperature data.

### Other Input Data

SMOKE-BEIS2 requires either gridded or county-based land use data. Gridded land use data at a 4 km resolution were developed specifically for the SMRAQ application. These land use data were derived in part from the county-based land use data used in most current UAM-BEIS2 modeling,<sup>3</sup> land use data derived from the Advanced Very High Resolution Radiometer (AVHRR) satellite at 1.1 km resolution, and 1990 census data. The county-based land use covers only the United States, so the satellite data along with some Canadian agricultural census data were used for the Canadian grid cells. The 1990 census data were used to identify urban and rural areas to help allocate urban and rural land use types. The land use data were aggregated from 4 km to 36 km for application with SMOKE-BEIS2 to the SMRAQ domain.

Two emission factor tables are currently available for use with UAM-BEIS2: a “winter” table and a

“summer” table. These same tables can be used with SMOKE-BEIS2. The biogenic emission factors were adapted from Geron et al.,<sup>7</sup> Guenther et al.,<sup>10</sup> and Novak and Pierce.<sup>11</sup> The winter data are based on the assumption that deciduous vegetation can be mostly ignored and the summer data are based on the assumption of full leaf biomass conditions.

## **MODELING ISSUES**

This section discusses the modeling issues that we addressed during the application of SMOKE-BEIS2 for the SMRAQ project. The issues include how best to apply the meteorological data and the emission factor tables for use in SMOKE-BEIS2. The meteorological data considered include temperature, net solar radiation reaching the ground, and cloud data.

### **Meteorological Input Issues**

During the OTAG modeling effort, analysis indicated that biogenic emissions can be significantly different when using prognostic meteorological fields instead of observational meteorological fields in UAM-BEIS2.<sup>12</sup> The OTAG modeling effort used meteorological data from a prognostic meteorological model to drive the atmospheric chemistry model, but used observational meteorological data to estimate biogenic and motor vehicle emissions. For the SMRAQ modeling effort, we wanted to use consistent meteorological fields for both the emissions and atmospheric chemistry models.

#### **Temperature effects**

MM5 creates a three-dimensional, gridded temperature field and a two-dimensional, gridded “ground temperature” field. In most previous applications of UAM-BEIS2, observational data were from the National Weather Service (NWS). The NWS temperature data is typically measured at a height of 1.5 meters from the ground. Thus, we initially attempted to interpolate to get a temperature at 1.5 meters, but later realized a more logical approach was to use the temperature that best represented the temperature appropriate for BEIS2. We discussed the appropriate biogenic emissions input temperature with an expert,<sup>13</sup> and we concluded that: (1) the temperature expected by BEIS2 is the leaf temperature with adjustments from canopy shading; and (2) a height of 10 meters would, on average, best represent these leaf temperatures for seasonal biogenic emissions modeling. The height of the first layer in the SMRAQ configuration is 38 meters, thus the midpoint is 19 meters for the first layer. So a 10 meter temperature can not be directly generated from the MM5 configuration. However, the discussions with MM5 experts subsequently yielded another option of the “ground temperature”,  $T_g$ , which actually is the temperature at the top of the canopy, when a canopy exists<sup>14</sup>. Since this is the closest available temperature to that experienced by the vegetation, and since temperatures cannot be interpolated closer to the ground if no actual ground temperatures are available we decided to use the  $T_g$  from MM5.

#### **Cloud effects**

MM5 has several different cloud mechanisms available for simulating clouds on a regional scale. SMOKE-BEIS2 accepts inputs from three different MM5 cloud mechanisms as well as from observational data. For the SMRAQ project, the Kain-Fritsch (KF)<sup>15</sup> and Kuo<sup>16</sup> cloud mechanisms were investigated through sensitivity runs with the MM5. We compared the predicted clouds to NWS cloud observations and satellite data and determined that the KF mechanism performed the best; consequently, this mechanism was used for the seasonal simulation.

In most of the previous applications of UAM-BEIS2, NWS observational cloud data has been used to estimate cloud top and bottom height, and cloud fractional coverage. Then, UAM-BEIS2 uses these cloud estimates to calculate the net radiation that reaches the ground. For the SMRAQ project, MCIP outputs an estimate of cloud top and bottom height, and cloud fractional coverage for each grid cell. Similarly to the UAM-BEIS2, the SMOKE-BEIS2 code must calculate the solar zenith angle and use gridded MM5 pressure fields to derive an attenuation factor based on the estimated cloud information. This attenuation factor is

used to calculate the net radiation reaching the ground. Most of these calculations are already made during the MM5 execution. Rather than recalculate this information using the estimated cloud information and possibly introduce some error, we decided to use the net radiation reaching the ground (RGRND) directly from the MM5. RGRND is calculated but not output in version 1 of MM5, so some minor code changes were made to MM5 to output RGRND for use in SMOKE-BEIS2.

## Other Input Data Issues

Since the SMRAQ episode includes May and September, we considered whether the winter emission factor table should be used during these months. We thought it was possible that the northern part of the SMRAQ domain was cool enough to warrant use of the winter table. A previous BEIS2 application<sup>3</sup> used the average frost date for a certain county to determine if the winter table should be used or not. Based on that work, we decided to analyze the  $T_g$  fields generated by MM5 for May to see if any grid cells dropped below 0 °C. We found that a few cells in southern Canada for a few hours during one day fell below the freezing temperature between May 15-May 31. Considering this information, we decided to use the summer table for the entire simulation.

The land use data was developed externally for the SMRAQ simulation. The issue of how this gridded land use data compared to other land use data was explored. The North Carolina Department of the Environment and Natural Resources in North Carolina (NCDENR) wanted to use a sub-domain of the SMRAQ land use data for input into SMOKE-BEIS2 for an urban scale air quality modeling project. So, we compared the land use data for the NCDENR domain (NC and surrounding states only) to the county land use data used in most previous applications of UAM-BEIS2. To accomplish this, we added reporting capabilities to SMOKE-BEIS2 that allow the user to produce county total emissions before the environmental corrections are applied. We found that the gridded land use data in the NCDENR domain consistently produced 3-5% less VOC and NO emissions than the county land use data. This difference was explained by the different map projections used to obtain the land use data sets. The Lambert projection of the SMRAQ domain does not capture the total area in a county as well as the Albers projection used in the county land use data set. The further away the grid cells are from the center of the Lambert projection, the worse the area is properly represented. Given the high level of uncertainty with the land use data sets, we decided that the SMRAQ land use data set was satisfactory for use in the SMRAQ and NCDENR applications.

## RESULTS

Figure 2 shows the magnitude of daily NO and VOC species base-case biogenic emissions for all days of the seasonal episode. Isoprene is the dominant species throughout the simulation for the SMRAQ domain. Daily isoprene emissions ranged from 50-200 thousand tons during the summer. Paraffins varied from 20-50 thousand tons, while the other species varied little in comparison. Figure 3 illustrates the modeled temporal variation of RGRND and temperature during the simulation. The temperatures in Figure 3 are at a height of  $T_g + 1.5$  meters. This temperature was estimated by interpolating between the first layer temperature and  $T_g$ . This was the typical method used when comparing temperature data in previous MM5 simulations. Using this comparison, we found that the MM5 temperatures were generally 1 to 2 °C cooler throughout the simulation than what was observed. The peak biogenic emissions periods occurred during the high temperature periods of July 12-15, July 29-31, and August 16-18. Other periods of interest include June 31-July 4, July 21-23, and August 3-5 where isoprene emissions were lower due to more cloud cover and lower temperatures.

Table 1 compares state totals of SMRAQ isoprene emissions versus the 1995 OTAG isoprene emissions for July 10-16. These comparisons were carried out on states that were fully contained in both domains. Generally, OTAG isoprene emission estimates are 5-13% higher than the SMRAQ emissions. This can be explained by the slightly cooler SMRAQ temperatures, the use of prognostic cloud data in SMRAQ, and differences in the land use data sets.

Figure 4 presents results from SMOKE-BEIS2 while using three different options available to the user. The options used are the no clouds (NOCL), the RGRND, and the KF cloud data options. The no clouds (NOCL) option displays the isoprene emissions if clear skies were assumed. The cloud fraction is set to zero, then the solar angle is computed and net radiation reaching the ground calculated within SMOKE-BEIS2. The RGRND option is the option used for the actual SMRAQ simulation. This option uses the net radiation reaching the ground data directly from the MM5. The KF cloud data option uses the estimated cloud top and bottom height, and cloud fractional coverage output from MCIP as input into SMOKE-BEIS2. All options used the same gridded ground temperature data. These options were used to better understand the cloud contribution to the estimation of isoprene emissions.

The NOCL shows that the cloud attenuation reduced isoprene emissions from around 3% (e.g., June 13-15) to the 25% (e.g., May 28-30) range during the SMRAQ simulation. The isoprene emissions estimated from the use of the estimated cloud data from the KF mechanism are consistently lower than the emissions produced using RGRND directly from MM5. The reduction in emissions ranged from 3 to 35%. This difference can be explained by (1) the estimation of a cloud top and bottom height and cloud fraction for an entire 36km resolution grid cell and to a lesser extent (2) the shallow convective clouds in MM5 were not included in the calculation of RGRND. The latter was discovered after the completion of the SMRAQ simulation. The general temporal pattern is maintained with all of the options illustrating that temperature effects on isoprene emissions are more important.

## SUMMARY AND CONCLUSIONS

The estimation of biogenic emissions for the summer season of 1995 dealt with many important input data issues. The output from the prognostic meteorological model, MM5, provides a variety of input data for SMOKE-BEIS2. We solicited advice to fully understand how to use the MM5 data to provide input for SMOKE-BEIS2. Based on this advice and sensitivity runs using different input data, the ground temperature,  $T_g$ , and the net radiation reaching the ground, RGRND, were used as inputs into the SMOKE-BEIS2. We decided not to use the winter emissions factor table in addition to the summer table by examining  $T_g$  fields from May 15-31 to see the frequency of when  $T_g$  fell below 0 C. This condition occurred only a few hours in southern Canada during the 17 day period.

Isoprene emissions ranged from 50-200 thousand tons for the entire domain during the seasonal simulation. Paraffins varied somewhat in comparison with isoprene emissions, while the remaining CB-IV species varied relatively little over the entire simulation. The peak biogenic emissions periods occurred during the high temperature periods in mid and late July, and mid August, while the periods of low emission rates occurred during periods of cooler temperatures and more cloud cover in late June, early and late July, and early August. Comparisons with OTAG biogenic isoprene emissions revealed that during the period of July 10-16, daily OTAG emissions tended to be 5-13% higher than the SMRAQ emissions. This difference can be explained by the use of slightly cooler SMRAQ temperatures, prognostic cloud data, and differences in the land use data sets.

We used SMOKE-BEIS2 to simulate isoprene emissions with and without clouds. We found that the variation in cloud attenuation over the seasonal simulation reduced emissions from between 3 and 25%. Another SMOKE-BEIS2 option was used to incorporate KF cloud data when calculating isoprene emissions. The isoprene emissions using the KF cloud data were 3-35% less when compared with using RGRND directly from MM5. This difference was most likely caused by the estimation of cloud top and bottom height and cloud fraction on a regional scale for use in SMOKE-BEIS2 and to a lesser extent the shallow convective clouds are not included in the estimation of RGRND in MM5.

If future biogenic emission modeling continues to use prognostic meteorological data, such efforts should include seeking expertise on the variety of output data available when using a certain meteorological model. The SMRAQ effort demonstrated that the isoprene emissions from SMOKE-BEIS2 can vary up to 35% per day when using different meteorological data from MM5.

The temporal variability in biogenic emissions throughout the summer of 1995 was mainly driven by the temperature variation. Perhaps the overall seasonal variability is not captured by using emission factors for only the winter and summer. SMOKE-BEIS2 was applied in a real-time air quality modeling application<sup>17</sup> in the summer 1998 that included simulations in October. More future air quality modeling applications may involve the spring and fall seasons. Ideally, it may be better to have some transitional emission factors or other input data that describe the amount of living leaf biomass on a monthly or seasonal basis.

Our final suggestions are that future biogenic modeling systems should be flexible enough to more readily use future improvements in prognostic cloud mechanisms, and be able to speciate emissions for all future chemical mechanisms in air quality models. We found it helpful and therefore recommend that future modeling systems produce reports that allow the user to quality assess land use data, isolate cloud and temperature contributions, and produce hourly and daily county emissions totals.

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State	OTAG ISOP 7/10/95	SMRAQ ISOP 7/10/95	PDIFF 7/10/95	OTAG ISOP 7/11/95	SMRAQ ISOP 7/11/95	PDIFF 7/11/95	OTAG ISOP 7/12/95	SMRAQ ISOP 7/12/95	PDIFF 7/12/95	OTAG ISOP 7/13/95	SMRAQ ISOP 7/13/95	PDIFF 7/13/95	OTAG ISOP 7/14/95	SMRAQ ISOP 7/14/95	PDIFF 7/14/95	OTAG ISOP 7/15/95	SMRAQ ISOP 7/15/95	PDIFF 7/15/95	OTAG ISOP 7/16/95	SMRAQ ISOP 7/16/95	PDIFF 7/16/95	OTAG ISOP 7/16/95 ALL
AL	9524	8120	15	12993	10845	17	13817	13157	5	12184	11274	7	11807	11368	4	11592	10151	12	12286	10875	11	84203
AR	13953	14957	-7	14785	15288	-3	16098	15475	4	15924	15680	2	14603	11786	19	12777	10344	19	11717	11329	3	99857
CT	498	304	39	191	206	-8	362	418	-15	698	601	14	1265	909	28	1149	1049	9	521	394	24	4684
DE	108	111	-3	121	90	26	166	135	19	204	139	32	262	161	39	313	154	51	113	121	-7	1287
DC	6	15	-150	7	14	-100	8	18	-125	10	20	-100	13	27	-108	14	33	-136	7	14	-100	65
GA	9946	7814	21	11111	9983	10	11149	8964	20	9526	9446	1	9609	8338	13	10640	9666	9	11557	11126	4	73538
IL	1935	2314	-20	2521	2631	-4	3169	3276	-3	3674	3543	4	3572	3326	7	2751	2444	11	2590	2305	11	20212
IN	1361	1488	-9	1767	1969	-11	2154	2328	-8	2611	2437	7	2765	2784	-1	1585	2201	-39	1743	1574	10	13986
KY	4305	2964	31	5099	5605	-10	5901	6456	-9	6629	6096	8	5739	7046	-23	5295	5819	-10	5033	5904	-17	38001
LA	7916	7432	6	7677	8315	-8	8410	8057	4	7432	7020	6	5058	4656	8	4195	4674	-11	5357	5229	2	46045
MD	810	778	4	1017	723	29	1222	913	25	1505	1122	25	1908	1439	25	2200	1715	22	1023	809	21	9685
MA	847	437	48	217	292	-35	572	572	0	1235	887	28	2314	1469	37	1710	1336	22	934	685	27	7829
MI	2076	2125	-2	3221	3045	5	3587	3806	-6	5040	4278	15	6726	4089	39	3314	2444	26	1653	1485	10	25617
MS	8833	7859	11	10486	10327	2	11756	12565	-7	10851	10578	3	8732	10321	-18	9196	7462	19	10039	8740	13	69893
MO	10161	13353	-31	14369	13393	7	17573	16369	7	18556	17545	5	16973	15311	10	15245	13267	13	13747	12004	13	106624
NH	538	331	38	192	356	-85	473	540	-14	1060	867	18	1721	1166	32	660	954	-45	699	656	6	5343
NJ	719	703	2	580	476	18	846	635	25	1240	918	26	1701	1119	34	2151	1453	32	678	916	-35	7915
NY	1207	730	40	1078	702	35	1494	1303	13	2514	2262	10	3362	2849	15	2962	2259	24	1534	1304	15	14151
NC	5414	6118	-13	6302	6590	-5	7040	6984	1	6857	6266	9	7583	6925	9	8362	7493	10	6724	5997	11	48282
OH	1369	1030	25	1633	1425	13	2011	1894	6	2641	2137	19	2492	1572	37	2636	2407	9	1884	1884	0	14666
PA	3275	2537	23	3295	2576	22	4853	3884	20	6273	5272	16	8328	7909	5	10177	8507	16	4601	3928	15	40802
RI	205	151	26	53	86	-62	120	165	-38	249	215	14	524	390	26	450	439	2	215	175	19	1816
SC	4470	4069	9	4722	3752	21	4448	4775	-7	4161	3945	5	3590	3564	1	4432	3703	16	5003	4411	12	30826
TN	6360	4803	24	7652	7901	-3	8570	9071	-6	8970	9140	-2	8217	8212	0	6937	6114	12	7162	6973	3	53868
VT	237	160	32	171	213	-25	341	381	-12	599	541	10	865	557	36	309	438	-42	298	368	-23	2820
VA	5352	5248	2	6587	5963	9	7269	5684	22	8411	7129	15	9857	8599	13	11374	9377	18	7158	4211	41	56008
WV	2831	2201	22	3510	2761	21	4057	3002	26	4825	4227	12	4811	3643	24	6212	4740	24	3660	3935	-8	29906
WI	4128	3657	11	5634	5310	6	5631	4458	21	10130	7090	30	9224	5867	36	3157	2274	28	1993	2343	-18	39897
Total	108384	101809	6	126991	120837	5	143097	135285	5	154009	140675	9	153621	135402	12	141795	122917	13	119929	109695	9	947826

**Table 1.** State isoprene emissions for July 10-16, 1995. SMRAQ versus OTAG with PDIFF being the percentage difference, (OTAG - SMRAQ)/OTAG .



Figure 1. SMRAQ modeling domain

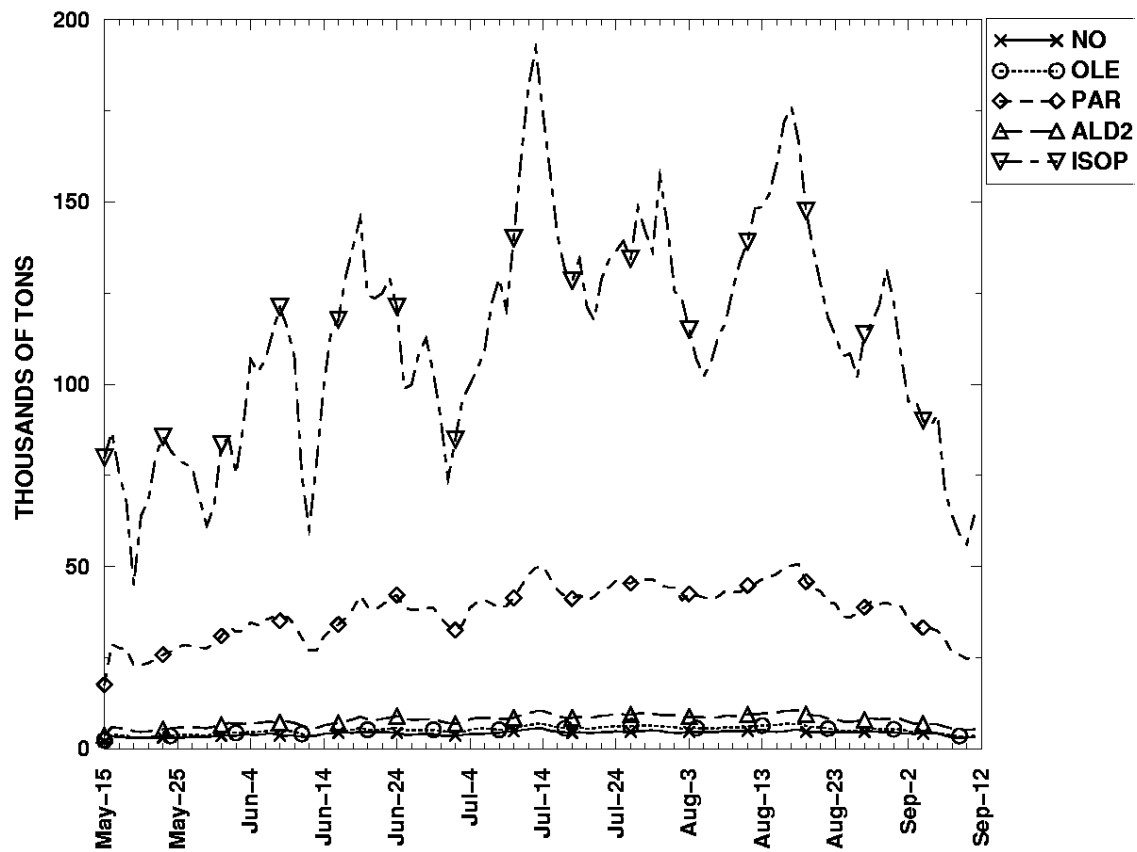
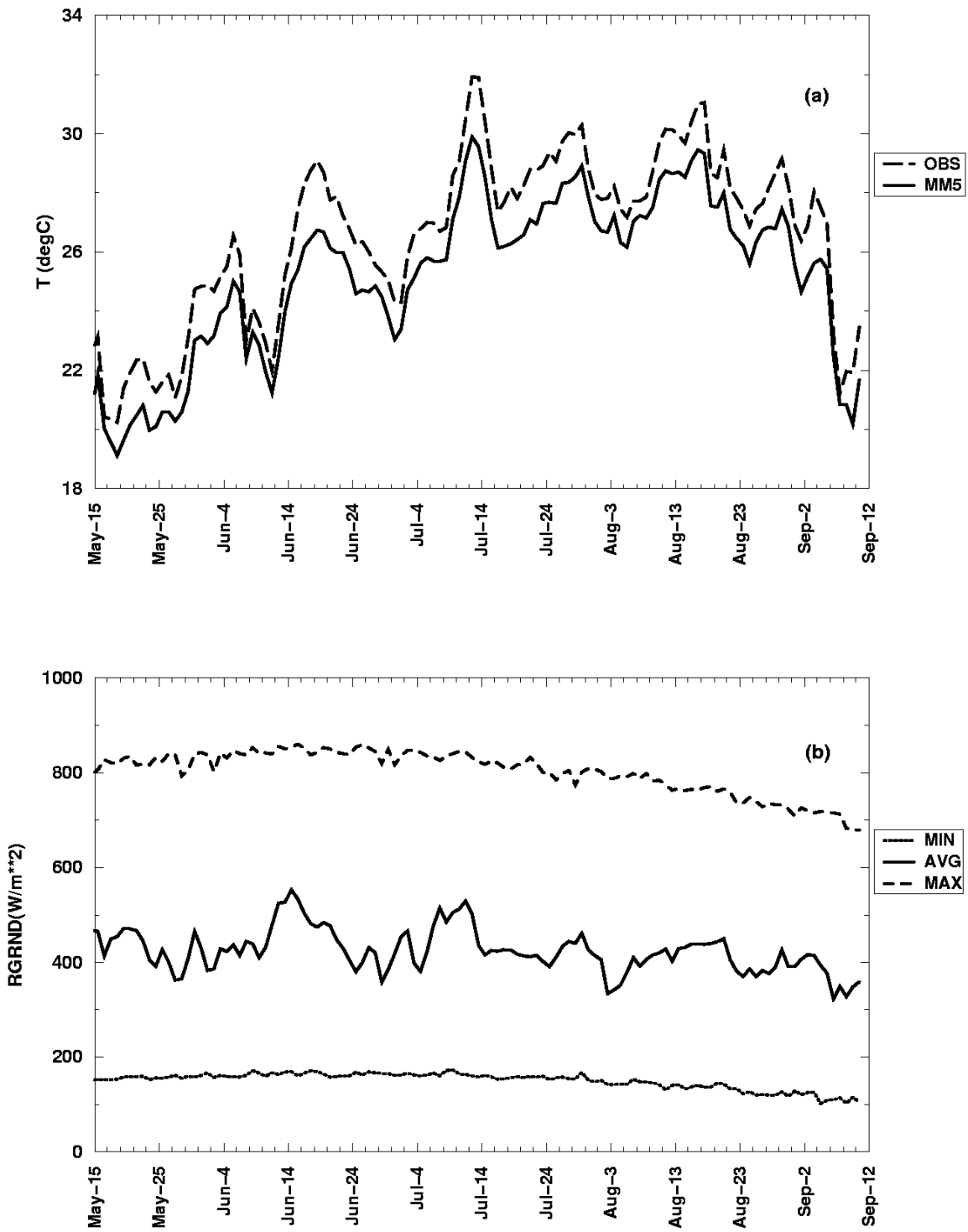
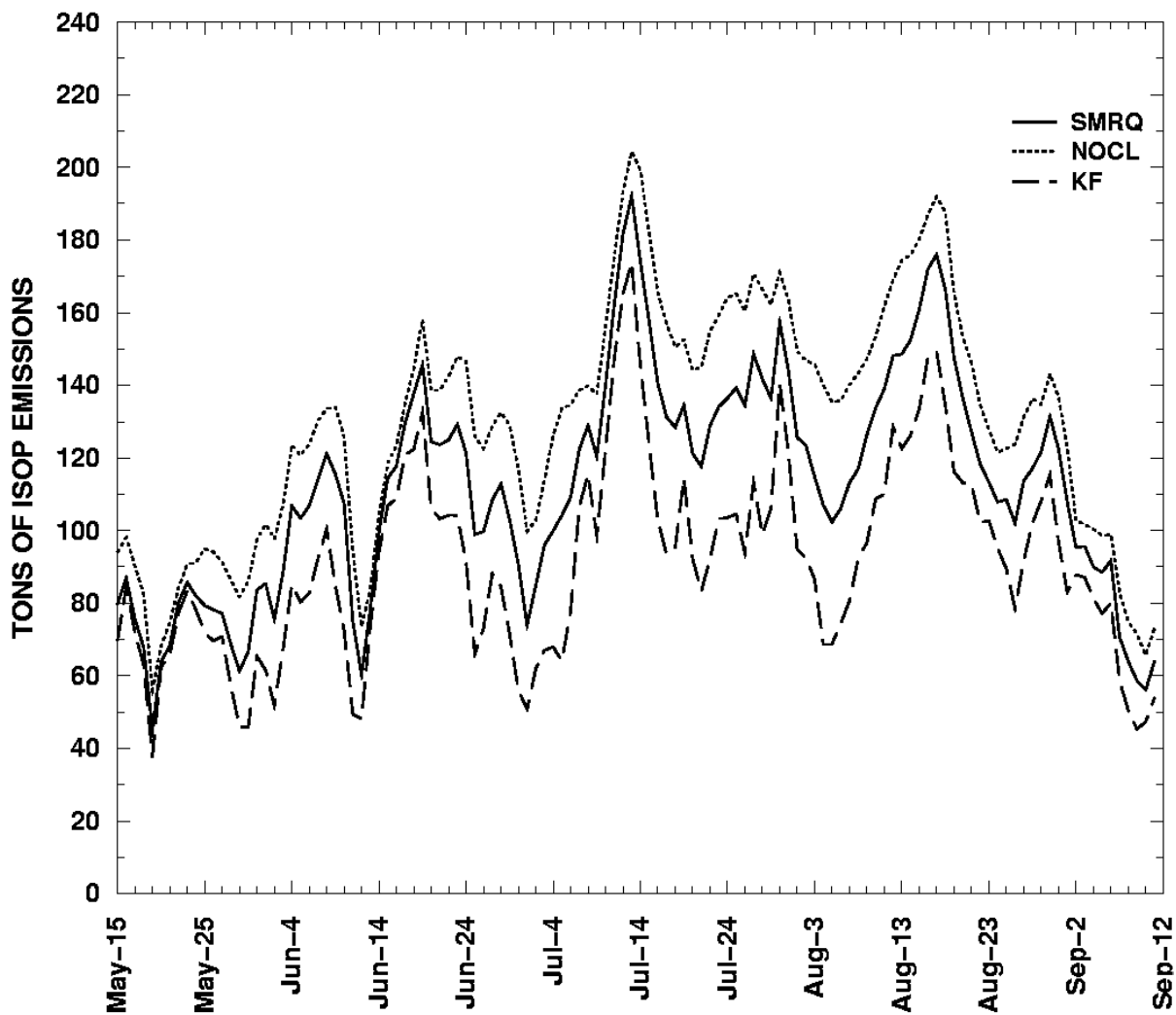


Figure 2. SMRAQ daily biogenic emissions for the summer of 1995



**Figure 3.** Average MM5 temperature versus observed temperature (a) and average MM5 net radiation reaching the ground (b) during the 1995 SMRAQ simulation. The average maximum, overall average, and average minimum net radiation reaching the ground (RGRND) are plotted.



**Figure 4.** Comparison of daily isoprene emissions totals where SMRQ is the emissions used in the SMRAQ application, NOCL is the emissions if clear skies is assumed, and KF is the emissions when the output from the Kain-Fritsch cloud mechanism is used to estimate cloud top and bottom height, and cloud fraction.

## KEYWORDS

biogenic, emissions, isoprene, air-quality, modeling, meteorology

