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Air Quality Modeling System Ⅰ

- Development of Emissions Preparation System with the CAPSS -

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FOREWORD

Developing an air quality modeling system has been deemed necessary to establish a control system for future state implementation plans and to understand how air pollutants can be effectively controlled in their emission, transport and reaction. In order to do so, it is important to predict three-dimensional meteorological field of the local area whose result can, in turn, help calculate emissions amount and build a photochemical reaction model to predict their influences on air quality.

It is important to note that the KEI-EIPS—developed by this study—is the first pre-emission treatment system that can be continuously upgraded through bug reports by its users. Moreover, it is not only open to use for the public, but also easy to use. Lack of any standardized tools, so far, has led to conflicting results despite having same emission data. Hopefully, the KEI-EIPS is expected to minimize disputes in predicting air quality and in planning mitigation strategies because it can be universally used and easily replicated so that national emission data can be available for any air quality simulation studies.

Lastly, I would like to express my sincere thanks to the authors, Nankyoung Moon, Soontae Kim and Daewon W. Byun for their efforts and hard work. Many people contributed to this study. I owe special thanks to Professor Yong Pyo Kim, Dr. Jae Cheol Nam, Professor Young-Kee Jang, and Professor Chong Bum Lee for their helpful comments and suggestions.

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Abstract

In order to properly estimate changes in air quality associated to national, regional, urban, and local development plans and to correctly explain the source-receptor relationship as of now, it is required to prepare most updated inputs to air quality modeling assessment or prediction. In current air quality assessment plans, it is not intensively considered to estimate the environmental capacity based on total amounts of aggregated emissions rates for a modeling region of interest. However it is necessary in the near future to assess or calculate environmental capacity to introduce an aggregated regulation on emissions rates for a targeted region in response to a future plan. In addition to predict impacts of secondary air pollutants such as ozone or Particular Matter on local air quality in Preliminary Environmental Review System (PERS) and Environmental Impact Assessment (EIA), it needs to predict three-dimensional meteorological filed of the local area, and, by using its result that, in turn, helps calculate emissions amounts and build a photochemical reaction model to predict their influences on air quality.

At this moment the Clean Air Policy Support System (CAPSS; Korea emission inventory, 2001, 2002, 2003 released by the Ministry of Environment) becomes available to apply on the air quality modeling works for the exercise explained above. However, the CAPSS itself can not be used directly as inputs for air quality models. Thus it becomes urgent and important to develop a new tool which allows users to use the emissions inventory for their purposes.

In this project, we have developed Korea Environment Institute-Emissions Inventory Preparation System (KEI-EIPS) to generate air quality model-ready emissions data with SMOKE (Sparse Matrix Operator Kernel for Emissions) using the Ministry of Environment's emissions inventory data, maintained under the Clean Air Policy Support System (CAPSS) database.

To utilize the SMOKE system, CAPSS SCCs were linked to US EPA's SMOKE default SCCs to the best match profiles for the chemical speciation, and the cross-reference tables and profiles for temporal and spatial allocations

since it is difficult to develop these internal databases in a short time characterizing all the SCCs used in the CAPSS. After examining emissions amounts for each source type, it is suggested to update internal databases for the top 10 SCCs for area and point sources and top 5 SCCs for on-road mobile sources first to minimize uncertainties during the emissions processing. Characterization on emissions sources should be carried out for a selected modeling region because each region presents different emissions patterns associated with different industrial, residential, and traffic environments.

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Chapter 1. Introduction

1. Background

In order to properly estimate changes in air quality associated to national, regional, urban, and local development plans and to correctly explain the source-receptor relationship as of now, it is required to prepare the most updated inputs to air quality modeling assessment or prediction. In current air quality assessment plans, it is not intensively considered to estimate the environmental capacity based on total amounts of aggregated emissions rates for a modeling region of interest. However it is necessary in the near future to assess or calculate environmental capacity to introduce an aggregated regulation on emissions rates for a targeted region in response to a future plan. In addition, to predict impacts of secondary air pollutants such as ozone or Particular Matter on local air quality in Preliminary Environmental Review System (PERS) and Environmental Impact Assessment (EIA), it needs to predict three-dimensional meteorological filed of the local area, and, by using its result that, in turn, helps calculate emissions amounts and build a photochemical reaction model to predict their influences on air quality.

At this moment the Clean Air Policy Support System (CAPSS; Korea emission inventory, 2001, 2002, 2003 released by the Ministry of Environment) becomes available to apply on the air quality modeling works for the exercise explained above, the CAPSS itself, however can not be used directly as inputs for air quality models. Thus it becomes urgent to develop a new tool which allows users to use the emissions inventory for their purposes.

Currently the CAPSS was provided with two types in terms of the data format; one is a database classified for each administrative area and the other is in a 1-km spatial resolution format in a TM (Transvers Mercator) coordination system. In case of the 1-km spatial resolution format in the TM coordination system, it was prepared to use pre-gridded emissions data in air quality models by the CAPSS developers. However, in general simulation domains for meteorology and air quality modeling are based on either Lambert-Conformal or Latitude-Longitude coordinates. The TM coordinate is

more proper for Gaussian models rather than Eurerian models, and emissons data previously gridded on a predefined map projection and a domain cell resolutiondomain become problematic when different map projection and resolution need to be used for a domain setup. For example, when spatially allocated emissions data at a 1-km resolution is used for air quality simulations for a region, it is difficult to apply regional growth and control factors for each source type and each emissions species to predict the response to a future plan, and to explain a source contribution to current air quality. For another example, the U.S. EPA releases the National Emissions Inventory to make it available to air quality modelers in a specified data format every 3 years. It is quite similar to the CAPSS emissions inventory, but more systematically organized to provide the users with more convenient access to it.

To resolve this problem and to provide an easy access to the CPASS emissions inventory, in this research it was designed to develop an emission preprocessing system capable of temporally and spatially allocating and chemically speciating the CAPSS emissions inventory for an air quality modeling work suitable to the user's approach.

The Ministry of Environment has implemented emissions processing methods to build emissions inventory (EI; CAPSS) for air quality research and policy decision in Korea. The emissions inventory data includes the country-specific information such as emission source classifications and characterizations. It prevents researchers from processing the emissions inventory with existing emissions processors such as the Sparse Matrix Operator Kernel for Emissions (SMOKE, Coats et al, 1995 and Benjey et al., 2001) and the Emissions Preprocessing System (EPS) to understand air quality better in the region and to help policy-making through air quality modeling works with U.S. EPA's Community Multi-scale Air Quality (CMAQ) modeling system.

One of the key scientific benefits of using the SMOKE system is that it allows easy extension of the chemical mechanisms, permitting investigation of the effects of the specific chemical components (e.g., highly reactive C2-C4 olefin species) on ozone production. With some additional efforts, the SMOKE system can be extended to include speciated particulate emissions

and air toxic species. The computational benefits of the SMOKE system include the ability to process emissions much faster than other systems, to minimize redundant data storage for decreased file sizes, and to provide outputs for the air quality models (AQM) such as CMAQ (Byun and Ching, 1999; Byun and Schere, 2006) and CAMx modeling systems.

In this project, we have proposed to develop the Korea Environment Institute-Emissions Inventory Preparation System (KEI-EIPS) to generate air quality model-ready emissions data with SMOKE using the MOE's emissions inventory data, maintained under the Clean Air Policy Support System (CAPSS) database.

2. Objectives

The main objective of this project is to develop efficient computational tools to convert the Korea emission inventory data into a data format accepted by the SMOKE emissions model to extend chemical speciation for a selected chemical mechanism such as SAPRC99 and CB4, to temporally allocate annual avarage day emissions into hourly resovled emissions, to have spatially allocated emissions for a tageted model domain in a resolution determined, and to check uncertainties in the Korea emission inventory through CMAQ simulations after SMOKE processing.

The current version of SMOKE is primarily an emission processing system and not an emission inventory preparation system. Its purpose is to provide an efficient tool for converting emissions inventory data into formatted emission files required by an air quality model (AQM). The sparse matrix approach utilized throughout SMOKE permits both rapid and flexible processing of emissions data. The processing is flexible because the processing steps of temporal projection, controls, chemical speciation, temporal allocation, and spatial allocation have been separated into independent operations wherever possible. KEI-EIPS based on SMOKE extends present air quality modeling capability to handle science research issues better in such areas as (1) including different chemical mechanisms, (2) processing additional chemical species for particulate matter and air toxics,

and (3) increasing multi-scale modeling efficiency needed for the studies involving the 8-hour ozone standard and PM modeling. This project is targeting to provide the first step able to process an emissions inventory processing tool for air quality studies.

The objectives of this project are: (1) implementing the CAPSS to the SMOKE system; (2) providing a method to generate domain-specific surrogates for spatial allocation in the Korean Peninsula, (3) setting up a cross-reference table between CAPSS and U.S. EPA source classification codes (SCC) for temporal allocation and chemical speciation, (4) processing the CAPSS for CMAQ simulations; (5) providing capability to generate inputs for testing emissions with different chemical mechanisms and inputs to the CMAQ air quality model; (6) providing capability to be extended to multiple pollutants, including particulate matters.

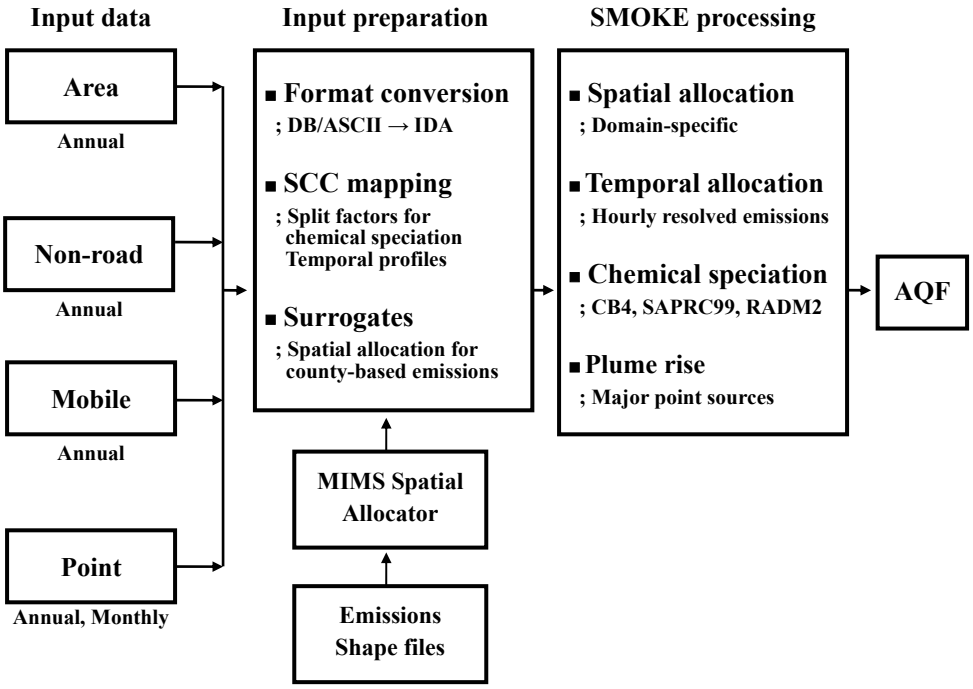

Figure 1.1 Schematic diagram showing how the CAPSS is linked to the SMOKE system. Emissions files in the CAPSS are reformatted to the SMOKE-ready format. A SCC mapping is used to have internal databases for temporal allocation and chemical speciation. A set of shape files is used to prepare spatial surrogates for a domain with the MIMS spatial allocator.

Chapter 2. Meteorology Simulation

1. MM5 Overview

The Fifth-Generation NCAR / Penn State Mesoscale Model is the latest in a series that was developed from a mesoscale model used by Anthes at Penn State in the early `70's that was later documented by Anthes and Warner (1978). Since that time it has undergone many changes designed to broaden its applications. These include (i) a multiple-nest capability, (ii) nonhydrostatic dynamics, and (iii) a four-dimensional data assimilation (Newtonian nudging) capability, (iv) increased number of physics options, and (v) portability to a wider range of computer platforms, including OpenMP and MPI systems. The purpose of this introduction is to acquaint the user with some concepts as used in the MM5 modeling system. Flow-charts of the complete modeling system are depicted in the schematic diagrams in Figure 2.1. It is intended to show the order of the programs, flow of the data, and to briefly describe their primary functions.

Terrestrial and isobaric meteorological data are horizontally interpolated (programs TERRAIN and REGRID) from a latitude-longitude grid to a meso-scale, rectangular domain on either a Mercator, Lambert Conformal, or Polar Stereographic projection. Since the interpolation of the meteorological data does not necessarily provide much meso-scale detail, the interpolated data may be enhanced (program LITTLE_R/RAWINS) with observations from the standard network of surface and rawinsonde stations using a successive-scan Cressman or multi-quadric technique. Program INTERPF then performs the vertical interpolation from pressure levels to the σ-coordinate of the MM5 model. Alternatively, program 3DVAR may be used to ingest data on model σ-levels. After a MM5 model integration, program INTERPB can be used to interpolate data from σ-levels back to pressure levels, while program NESTDOWN can be used to interpolate model level data to a finer grid to prepare for a new model integration. Graphic programs (RIP and GRAPH) may be used to view modeling system output data on both pressure and σ-levels.

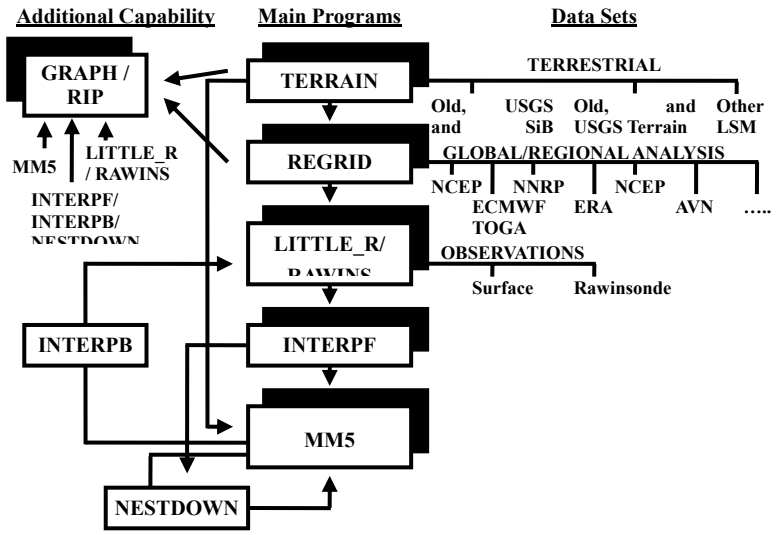

Figure 2.1 The MM5 modeling system flow chart.

2. Configuration

MM5 contains a capability of multiple nesting with up to nine domains running at the same time and completely interacting. The nesting ratio is always 3:1 for two-way interaction. "Two-way interaction" means that the nest's input from the coarse mesh comes via its boundaries, while the feedback to the coarser mesh occurs over the nest interior. Nests may be turned on and off at any time in the simulation, noting that whenever a mother nest is terminated all its descendent nests also are turned off.

In this study, MM5 is simulated during 29 May - 20 June, 2004 period and the one-way nested simulations with the 43 vertical levels in the atmosphere for the 27km, 9km, and 3km resolution domains centered for Seoul Metropolitan area were made. The modeling options used are; observation nudging with AWS and upper air observation, a counter-gradient planetary

boundary layer mixing scheme (so called MRF scheme), and the five-layer soil scheme model option. The nested domain was setup with 109 X 109, 82 X 82, and 70 X 70 for the resolution of 27km, 9km, and 3km, respectively. The initial field was selected NCEP/NCAR CDAS reanalysis data that is prepared by 6 hourly data for time resolution and 2 X 2.5 degrees data for the horizontal resolution. Other configuration details are presented in Table 2.1.

Table 2.1 The configuration of MM5 simulation.

	Domain 1	Domain 2	Domain 3
Horizontal Grid	109 X 109	82 X 82	70 X 70
Resolution	27 km	9 km	3 km
Vertical Grid	43 Layers		
Physical option	Grell cumulus Scheme		
	MRF PBL Scheme		
	Five-Layer soil Scheme		
Initial data	NCEP/NCAR CDAS Reanalysis Data		

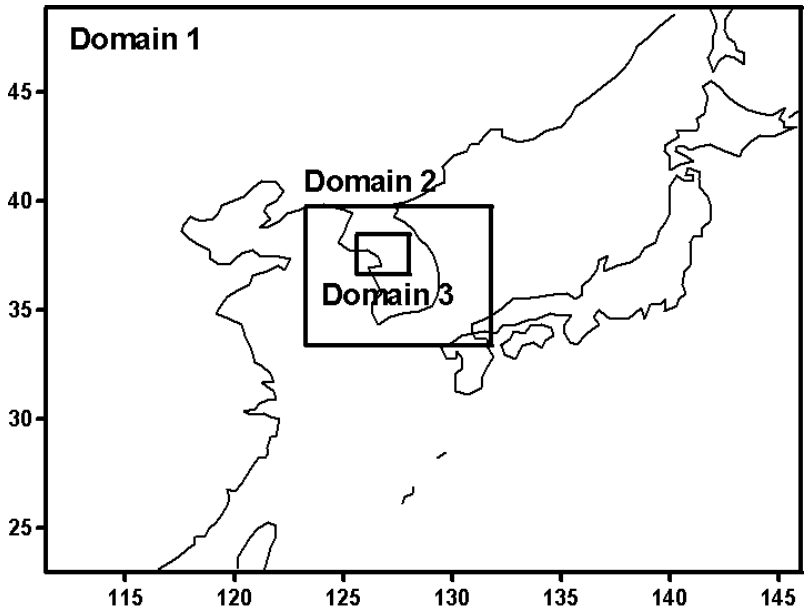

Figure 2.2 Modeling domain defined in MM5.

3. Comparisons of MM5 Results to the Observations

Meteorological field plays an important role in estimation of emission and air quality modeling. In processing of the emission field, meteorology data is used for plume rise process and biogenic emission processing. Advection and diffusion related with meteorology data are the most important things in air quality modeling

Figure 2.3 and 2.4 show the simulated and observed time series of temperature, wind speed and wind direction for surface station data as the results of MM5 of 3km resolution at Seoul and Icheon station, respectively. The observation nudging was conducted in the MM5 simulation to get better results. When we compare the simulated values to observed values for temperature, wind speed includes zonal and meridional values and wind direction, respectively, the simulated results shows good correlation for most cases.

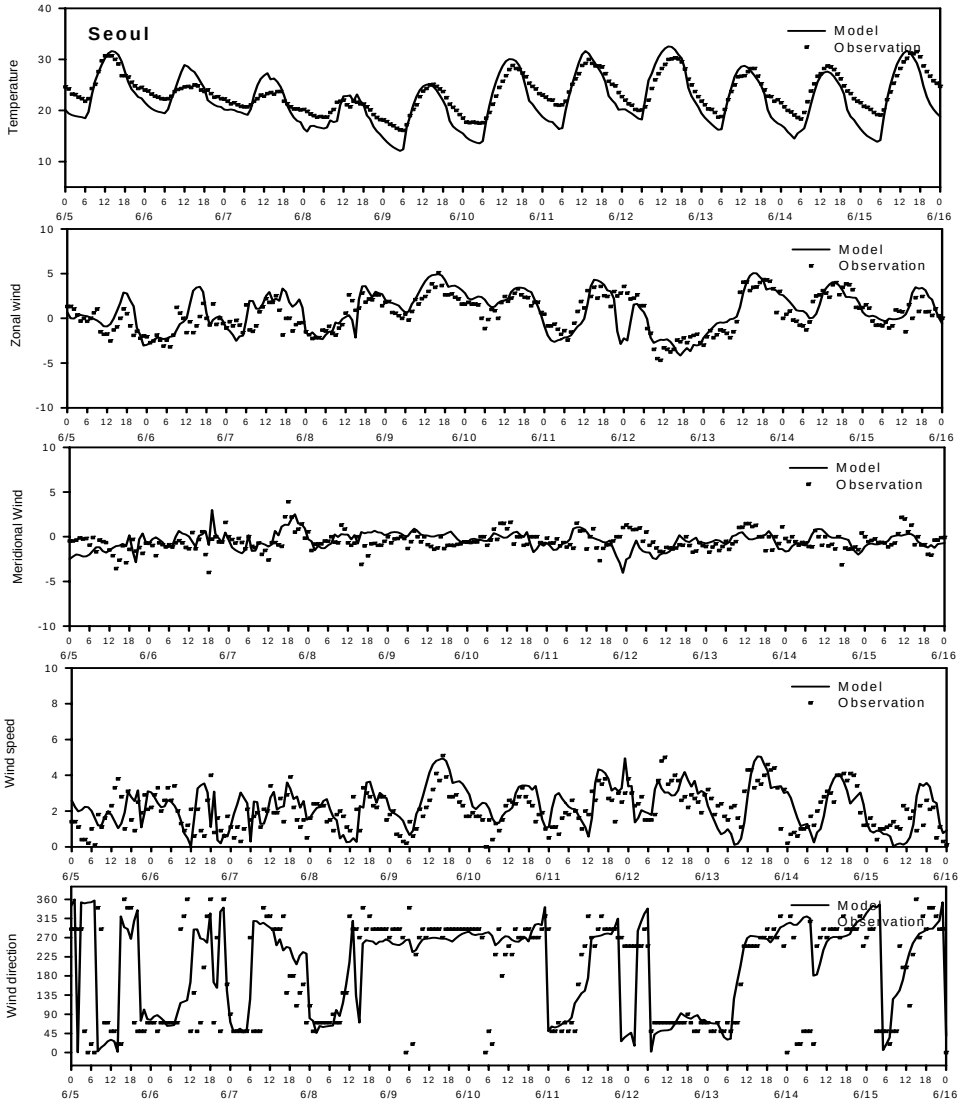

Figure 2.3 Simulated and observed time series of temperature, wind speed and wind direction for surface station as the results of MM5(3km) at Seoul station.

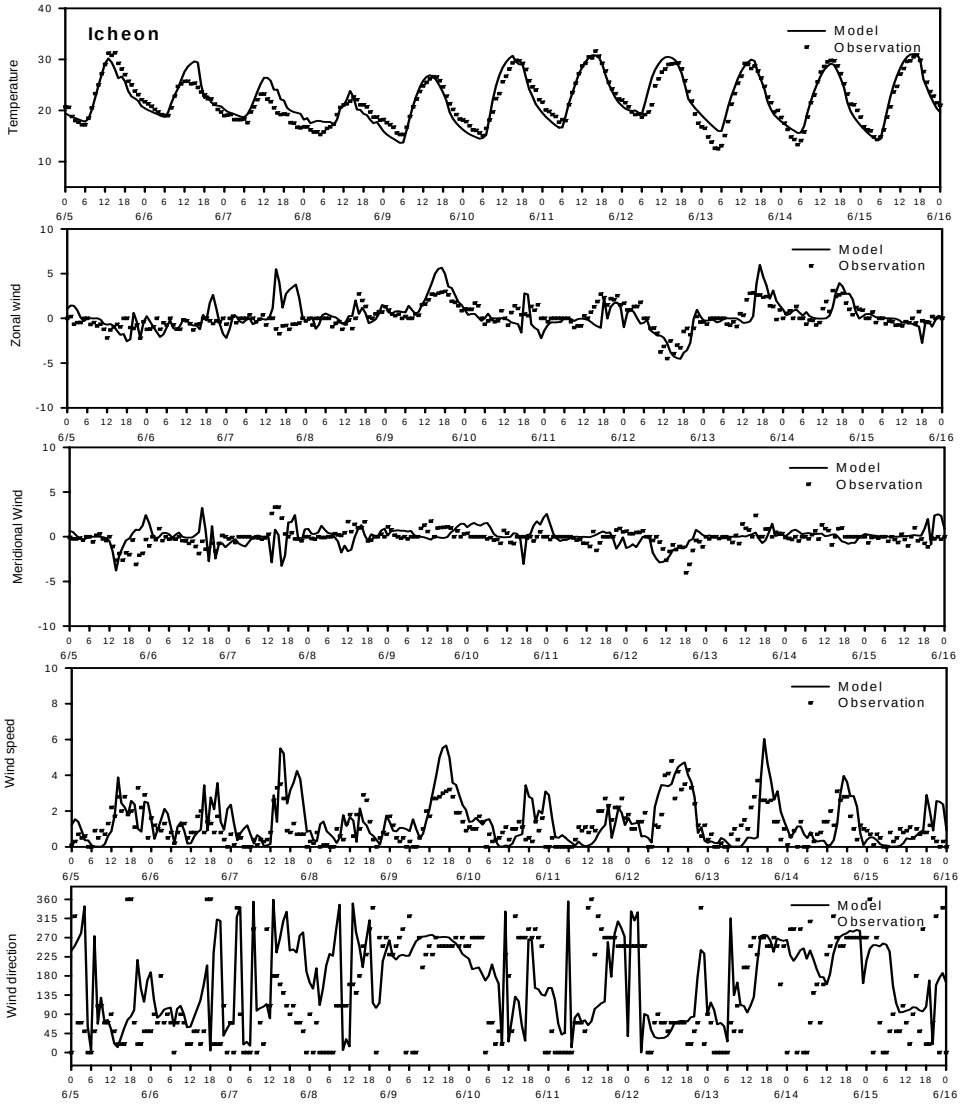

Figure 2.4 The same as Figure 2.3 except for Icheon.

Chapter 3. The CAPSS Emission Preparation System

1. CAPSS Emissions Inventory and Internal Data Bases

1.1 CAPSS Emissions Inventory

The CAPSS emissions inventory (EI) for year 2003 was used in this study. The EI was prepared as point and non-point emissions sources for seven criteria species; a) NOx, b) VOC, c) CO, d) NH_3, e) SO_2, f) PM10, and g) TSP.

Table 3.1 The CAPSS Emissions Inventory.

Source	EI category	Emission Type
Non-point emissions	Area	Annual,County-based, reclassified with SCC codes from non-point emissions
	Non-road mobile	Annual,County-based, reclassified with SCC codes
	On-road Mobile	Annual,County-based, reclassified with SCC codes
	Biogenic	Annual,County-based, reclassified with SCC codes from non-point emissions, Currently NH_3 only
Point emissions	All point sources	Annual and Month emissions, State-level. A TM map projection used

1.2. Emission Shape Files for Spatial Allocation

For spatial allocation of criteria pollutants emissions, a set of GIS shape files were acquired and processed with the MIMS spatial allocator. The SMOKE system does not have surrogates for Korea, and it is necessary to prepare surrogates for spatial allocation for a domain setup. The MIMS spatial allocator (http://www.cep.unc.edu/empd/projects/mims/spatial/) is a tool released by the U.S. EPA to prepare surrogates out of a set of shape files and land use land cover data for biogenic emissions.

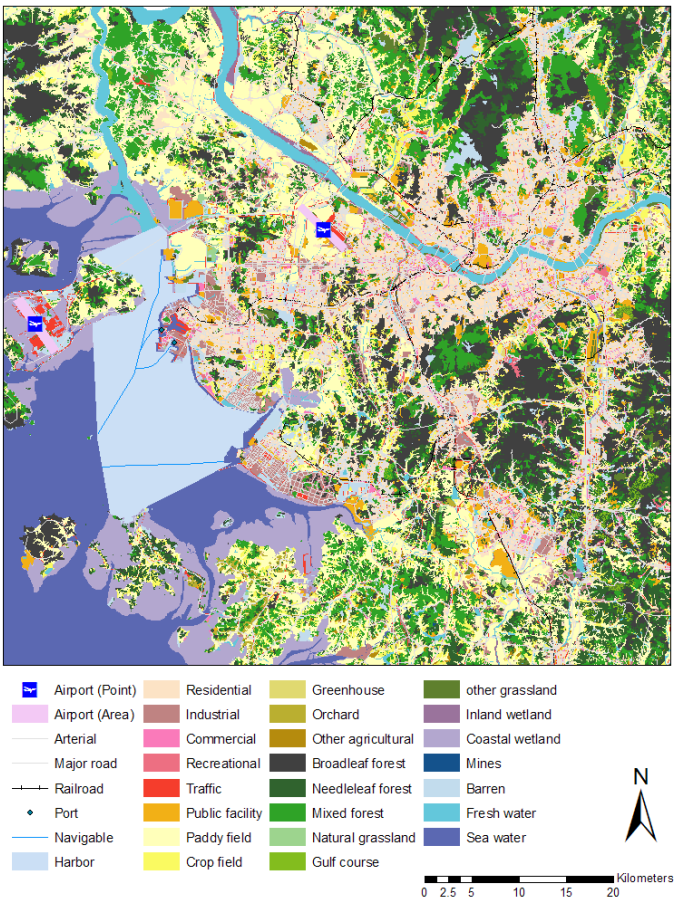

Figure 3.1 A set of shape files used to develop surrogates for spatial allocation in this study.

1.3. Internal Data for Chemical Speciation and Temporal Allocation for CAPSS

The same emissions inventory processed with emissions processing system such as SMOKE or EPS can result in different model-ready emissions because of their dependencies on the different cross-reference and profile files used for spatial and temporal allocations, and chemical speciation. During the SMOKE processing in this study, the default cross-reference and profiles implemented in SMOKE were used for chemical speciation and temporal allocation. To use the internal databases inside SMOKE for chemical speciation and temporal allocation, the Source Classification Code (SCC) needs to be properly assigned to the best-matching profile. Currently the U.S. EPA has prepared around 20,000 SCCs to describe an emission source with an assigned number. On the other hand, the CAPSS uses around 1,000 SCCs which uses an independent set of numbering system that does not match with the convention used by the U.S. EPA. Therefore, it was needed to map SCCs in the CAPSS to those in the U.S. EPA to use those internal databases for chemical speciation and temporal allocation as released without further revision of the SMOKE system. For this, it was assumed that similar emissions sources present the same temporal variation and chemical compositions even though the default databases were prepared for emissions sources in the North America, which was not validated for emissions sources in Korea.

1.4. Meteorological Data

For the SMOKE processing, we have prepared the meteorological data such as temperature at 1.5m, etc., with MCIP (Meteorology-Chemistry Interface Processor) using a set of MM5 (Mesoscale Model) simulations. These MCIP output files were used for plume rise of major point sources to allocate emissions vertically and used to estimate biogenic emissions.

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2. KEI-EIPS Development

2.1. Development of Surrogates for Spatial Allocation

2.1.1. MIMS Spatial Allocator Processing

In order to provide a set of spatial surrogates for a modeling domain, a spatial surrogate generator in the Multi-scale Integrated Modeling System(MIMS; http://www.cep.unc.edu/empd/projects/mims/spatial/) was used. Quality assurance of the acquired shape files was first conducted using the Arc GIS before they were used as inputs for the MIMS spatial surrogate generator before and after the processing. Figures 3.2 ~ 3.4 show some examples of shape files and gridded data over 3-km and 9-km resolution modeling domains.

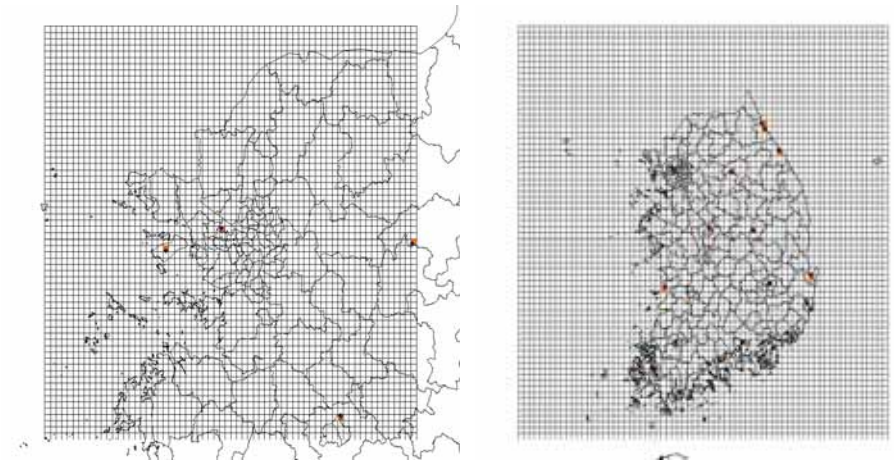


Figure 3.2 Airports gridded over 3-km (left) and 9-km (right) domains.

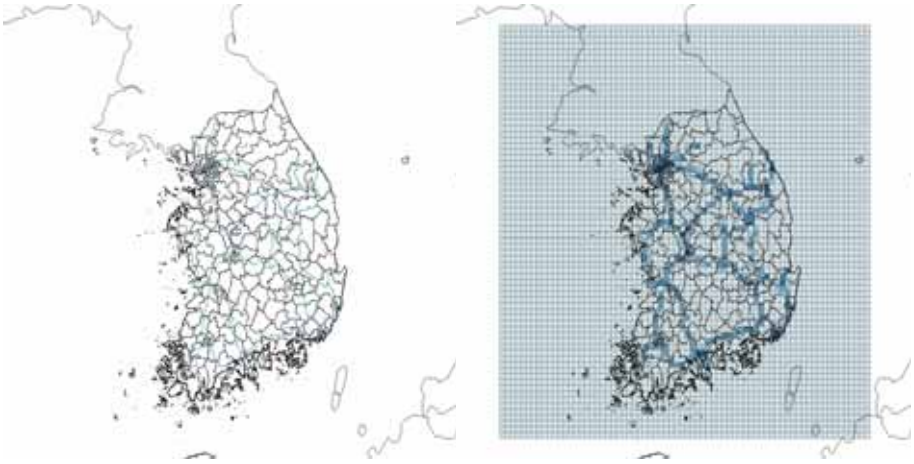


Figure 3.3 Railroad in a shape file (left) and gridded for a 9-km domain (right).

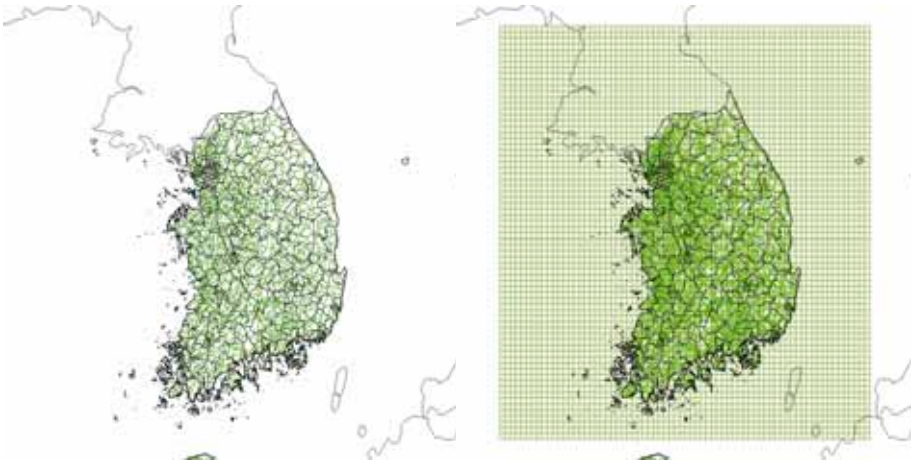


Figure 3.4 Road in a shape file (left) and gridded for a 9-km domain (right).

2.1.2. Surrogates Mapping for SMOKE Processing

Surrogates generated in the previous step were used in SMOKE processing to create the gridded emissions from county-based emissions such as area, non-road mobile, and biogenic emissions. In order to assign one surrogate for an emissions source, a cross-reference table for spatial allocation was used to properly distribute the emissions spatially inside SMOKE. It is very common to use the SCC of an emission source to assign the best matching surrogate. Table 3.2 presents the list of shape files available for Korea, which were processed with the MIMS Spatial Allocator in this study. After spatial allocations of shape files listed in Table 3.2, a combining step was used to generate one surrogtae by grouping a few shape files together as shown in Table 3.3.

Table 3.2 The list of shape files processed with the MIMS Spatial Allocator.

	Shape	Note
1	CITY_SiGunGu_01	City
2	AIRPORTS_02	Airport
3	POPULATION_03	Population
4	URBAN_ROAD_04	Urban road
5	LOCAL_ROAD_05	Local road
6	RAILROAD_06	Railroad
7	PORTS_08	Ports
8	WATERWAY_09	Waterway
9	RESIDENTIAL_11	Residential
10	INDUSTRIAL_12	Industrial

11	COMMERCIAL_13	Commercial
12	RECREATIONAL_14	Recreational
13	TRAFFIC_AREA_15	Traffic area
14	PUBLIC_FAC_16	Public facility
15	ARGI_PADDY_18	Agriculture, Paddy
16	ARGI_FIELD_19	Agriculture, Field
17	ARGI_GRNHOUSE_20	Agriculture, Greenhouse
18	ARGI_ORCHARD_21	Agriculture, Orchard
19	ARGI_OTHERS_22	Agriculture, Others
20	FOREST_DECI_25	Forest, deciduous
21	FOREST_CONI_26	Forest, coniferous
22	FOREST_MIXED_27	Forest, mixed
23	GRASS_NATURAL_29	Grass, natural
24	GRASS_GOLF_30	Grass, golf
25	GRASS_OTHERS_31	Grass, others
26	WETLAND_INLD_33	Wetland, In land
27	WETLAND_COAST_34	Wetland, coastal
28	MINES_36	Mines
29	BARREN_37	Barren
30	FRESH_WATER_39	Fresh water
31	SEAWATER_40	Seawater

Table 3.3 Shape files used to generate surrogates for SMOKE processing.

	Surrogates	Shape files
1	'AGRICULTURE_01'	Combine('ARGI_PADDY_18','ARGI_FIELD_19','AGRI_GRNHOUSE_20','AGRI_ORCHARD_21','AGRI_OTHERS_22')
2	'AIRPORTS_02'	'AIRPORTS_02'
3	'LAND_AREA_03'	'CITY_SiGunGu_01'
4	'HOUSEHOLDS_04'	'RESIDENTIAL_11'
5	'HIGHWAYS_07'	'LOCAL_ROAD_05'
6	'POPULATION_08'	'POPULATION_03'
7	'PORTS_09'	'PORTS_08'
8	'RAILROADS_10'	'RAILROAD_06
9	'NAVIGABLE_11'	'WATERWAY_09'
10	'RURAL_AREA_12'	(1–combine('RESIDENTIAL_11','INDUSTRIAL_12' 'COMMERCIAL_13''TRAFFIC_AREA_15' 'PUBLIC_FAC_16'))
11	'URBAN_AREA_13'	Combine('RESIDENTIAL_11','INDUSTRIAL_12''COMMERCIAL_13' 'TRAFFIC_AREA_15' 'PUBLIC_FAC_16')
12	'FOREST_14	Combine('FOREST_DECI_25','FOREST_CONI_26','FOREST_MIXED_27')
13	'URBAN_PRI_15'	'URBAN_ROAD_04'
14	'RURAL_PRI_16'	'LOCAL_ROAD_05'
15	'URBAN_SECND_17'	'URBAN_ROAD_04'

16	'RURAL_SECND_18'	'LOCAL_ROAD_05'
17	'URBAN_POP_19'	'POPULATION_03'
18	'RURAL_POP_20'	'POPULATION_03'
19	'COUNTY_60'	'CITY_SiGunGu_01'

2.2. Source Classification Code Mapping for Chemical Speciation and Temporal Allocation

2.2.1. Reclassification of the CAPSS Emissions Inventory for Each Source Type

As describe in Table 3.1, the CAPSS emissions inventory used in this study was prepared in two files formats; one for non-point sources and the other for point sources. To process emissions for each source type and to better match a SCC between the CAPSS and the U.S. EPA systems, the non-point emissions were reclassified to area, non-road mobile, onroad mobile, and biogenic emissions based on the first level SCC (SCC1) of emissions sources. Here, the first level SCC represents the first two characters used SCC as shown in Table 3.4. Description of the first level SCC (DESC1) and numbers of SCCs available for each SCC1 are also presented in the table. Currently, 803 SCCs are available from the CAPSS and they are mapped to those from the U.S. EPA(http://www.epa.gov/ttn/chief/codes/ index.html) as follows.

- Onroad Mobile = SCC1 of 07
- Non-road Mobile = SCC1 of 08
- Biogenic emissions = SCC1 of 10
- Area emissions = Others

Table 3.4 Descriptions and numbers of Source Classification Codes at the first level.

SCC1	DESC1	# of SCCs
01	Electric generating utility (EGU) combustion	34
02	Non-electric generating utility (NEGU) combustion	22
03	Industrial combustion	53
04	Industrial Processes	240
05	Storage and Transport	5
06	Solvent utilization	22
07	Onroad mobile	128
08	Non-road mobile	138
09	Waste treatment	26
10	Biogenic	103
11	Agriculture	32

2.2.2. Mapping of SCCs between the CAPSS and the U.S.EPA

During this step, SCCs for all the emissions inventory records in the CAPSS were mapped to those in the U.S. EPA, referring to the description of each SCC at levels 1 to 4. Here, level 1 means a major classification, and the higher levels represent more detailed classifications. Below is an illustration of a SCC mapping.

< CAPSS >

SCC	SCC_L1	SCC_L2	SCC_L3	SCC_L4
04051901	Industrial Processes	Chemical Manufacturing	Phthalic Anhydride	Point Source
04051902	Industrial Processes	Chemical Manufacturing	Phthalic Anhydride	Area Source

< SMOKE >

SCC	SCC_L1	SCC_L2	SCC_L3	SCC_L4
30101901	Industrial Processes	Chemical Manufacturing	Phthalic Anhydride	o-Xylene Oxidation: Main Process Stream
2301000000	Industrial Processes	Chemical Manufacturing: SIC 28	All Processes	Total

2.2.3. Limitations on the Current SCC Mapping

At this moment, SCC mapping between the CAPSS and the U.S. EPA was done for around 500 SCCs currently used in the CAPSS. While it is easy and straightforward for some SCCs in the CAPSS to find the corresponding SCCs from the U.S. EPA's list, there are other SCCs for which it is difficult to find well matched SCCs from the U.S. EPA. Also, there exist some possibilities to misinterpret descriptions for the SCCs during the mapping work. In such case, quite different SCCs in CAPSS could be mapped to the U.S. EPA's SCCs.

During emissions processing in the SMOKE system, a SCC is a key index to characterize the emissions source by assigning the best matching profile during each step of chemical speciation, temporal and spatial allocations.

Unfortunately, fuel types for boilers, and internal and external combustions were not included as a part of SCC in the CAPSS. Therefore, it is desired to include the fuel type, either by incorporating the fuel type in the SCC at the emissions inventory preparation step or by including them during a preprocessing step of the emissions inventory, similar to a format conversion, to have more detailed information on a source with a SCC assigned.

It would be necessary for a pool of experts to have intensive discussions to improve the emissions preparation steps by minimizing uncertainties associated with SCC mapping, source characterization for chemical speciation and temporal variation. Also, more detailed information inside the CAPSS would help understand source characteristics in the emissions inventory. Below are a list of a few points that need to be more discussed.

- How to improve the SCC mapping between the CAPSS and the U.S. EPA
- How to develop internal cross-reference tables and profiles for Korea
- What could be a "standard" format of the CAPSS emissions inventory to process for air quality modeling

2.3. The CAPSS Data Format Conversion to the IDA

It was required to convert the CAPSS emissions inventory to one of the SMOKE-ready formats prior to processing the emissions data. The SMOKE-ready CAPSS emissions inventory was then processed with SMOKE to provide CMAQ-ready emissions files to simulate ozone and particulate matter concentrations over Korea, and to quantitatively evaluate uncertainties in the data set after comparisons of the simulation results to observations. The analyses on SMOKE outputs can be used to feedback for updates in the emissions processing steps.

2.3.1. Non-Point Source Emissions

Emissions data from area, non-road and on-road mobile sources were

converted into the IDA format for area sources to have individual emissions records for each subregion such as Si, Gun, and Gu. Each record includes a FIPS code for each subregion, SCC, and emissions rates for each emission species. The CAPSS emissions inventory for these sources is available as the annual emissions rates, and the optional peak ozone day average emissions are assigned to be zero after the format conversion. The emissions species currently available are as follows;

- Header records for the IDA format from non-point source inventory.

```
#IDA
#TYPE       AREA Source Emissions Inventory
#COUNTRY    KOREA
#YEAR       2003
#DESC       CAPSS_V1_AREA
#DATA        CO        NOX       NH3       SOX       TSP       PM10      VOC
PM2_5
```

As of now, the PM2.5 emissions rates are not available from the CAPSS emissions inventory. However, it is essential to have the emissions to simulate particulate matter concentrations in air quality models. Therefore, an arbitrary factor of 0.5 was multiplied to PM10 emissions rates during the format conversion to have PM2.5 emissions rates. More discussions are necessary to develop the PM2.5 emissions inventory more correctly.

2.3.2. Point Source Emissions

For point sources, the IDA format for the point source inventory was used to convert the CAPSS. Unlike other source emissions, the CAPSS provides both annual and monthly emissions rates. Thus, in addition to annual emissions files for each species, monthly emissions rates files were separately prepared to have an option to process a proper point source emissions inventory based on a user's choice. Each emissions record includes a FIPS code, SCC, stack parameters such as stack height, stack diameter, temperature and exit velocity of exhausting gas for plume rise, and locations in latitude and longitude. If available, plant ID, point ID, stack ID, and plant name are

provided together.

- Header records for the IDA format from point source inventory (for example, NOx emissions)

```
#IDA
#TYPE        Point Source Emissions Inventory
#COUNTRY    KOREA
#YEAR        2003
#DESC        CAPSS_V1_POINT
#DATA        NOX
```

Chapter 4. Preliminary Evaluation on Emissions

After converting to a suitable format for SMOKE processing which includes the SCC mapping for chemical speciation, and temporal and spatial allocations, and developing the spatial surrogates for one 3-km and one 9-km resolution domains, the CAPSS emissions inventory was processed with SMOKE to test results of the emissions preparation system.

The emissions inventory was processed with the Carbon Bond 4 (CB4) chemical mechanism for the high ozone episode in 2004 (June 1st ~ June 15th). The 9-km resolution domain includes the whole area of South Korea, and the 3-km resolution domain encompasses the Seoul and Gyeonggi-Do as shown below. For the SMOKE processing, a set of MM5-MCIP outputs were used to vertically allocate major point sources, depending on the stack parameters and meteorology conditions. In this test run, a 23-layerd vertical structure was used, and the height of surface layer was ~ 33 meters.

Each processing step in SMOKE was explained with accompanying figures and tables in the following sections (section 1 ~ 4). In section 6, the CAPSS emissions inventory was evaluated with the SMOKE report files, which provide a summary of chemical speciation, temporal and spatial allocation results as well as the emissions inventory provided as inputs.

1. Spatial Allocation

Figures 4.1 and 4.2 represent spatial distributions of NOx emissions on the 9-km and the 3-km resolution domains from area, non-road mobile, on-road mobile, and point sources for June 11th, 2004 at 12 UTC. At this hour, on-road mobile sources contribute higher NOx emissions rates than other sources. As expected, NOx emissions rates from large cities such as Seoul and Busan are higher than other rural areas. For the 3-km resolution domain, NOx emissions from on-road mobile sources are predominant, which is followed by the non-road mobile and area sources over the Seoul

metropolitan area. Also, it is apparent that NOx emissions from Seoul and Incheon are much higher than other neighboring cities.

Similarly, on-road mobile emissions are the major source of ETH emissions. It can be seen there are high ETH emission from Seoul and Ulsan from area sources (Figures 4.3 and 4.4).

From Figures 4.5 and 4.6, it is shown on-road mobile sources contribute to most of PMFINE emissions. On the other hand, PMFINE emissions from non-road mobile sources are much lower than those from area sources.

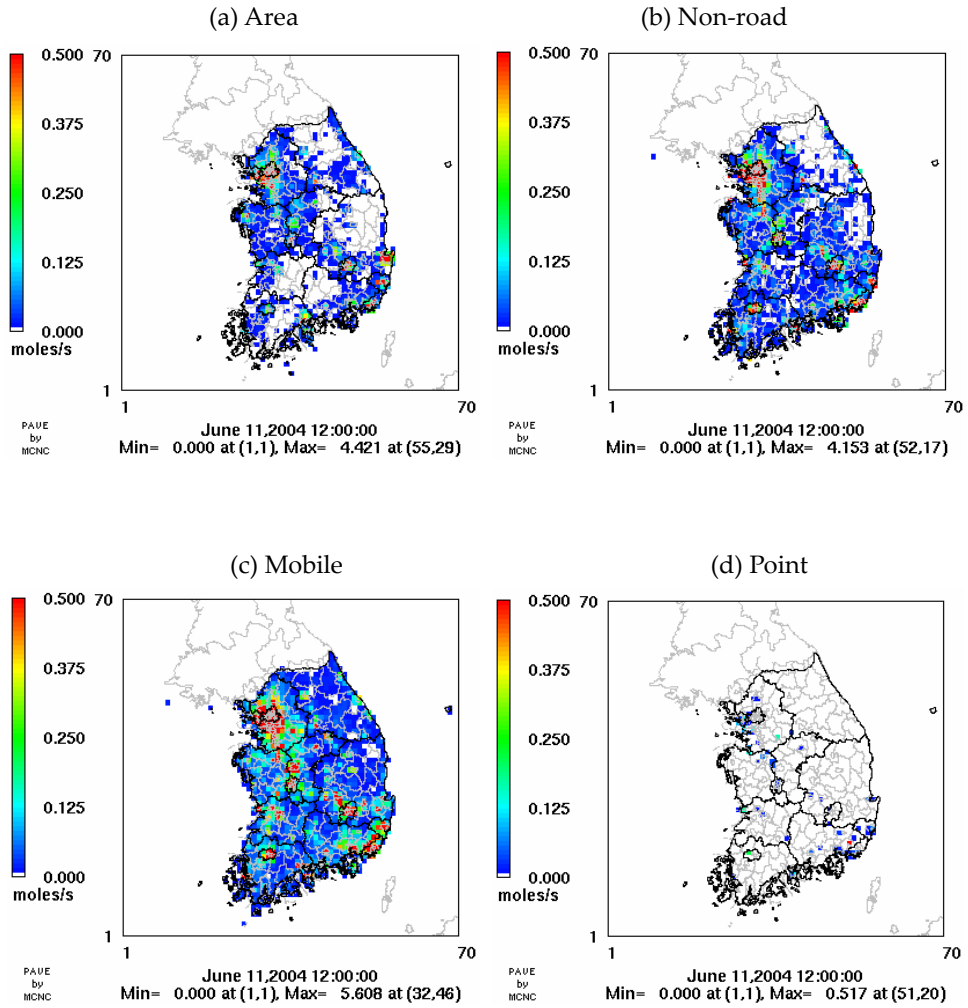
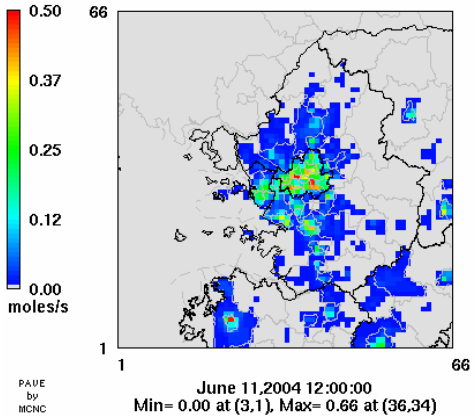
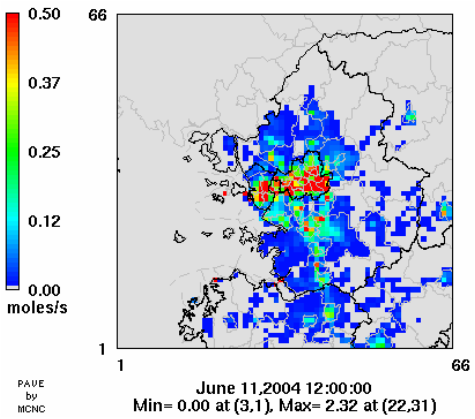


Figure 4.1 Spatial distributions of the CAPSS NO emissions processed by SMOKE for a 9-km resolution domain. For point sources, the emissions rates are shown for the surface layer only.

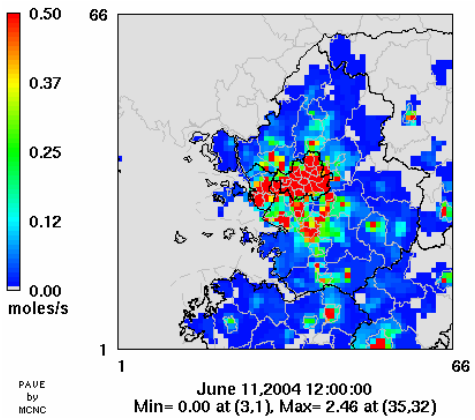
(a) Area



(b) Non-road



(c) Mobile



(d) Point

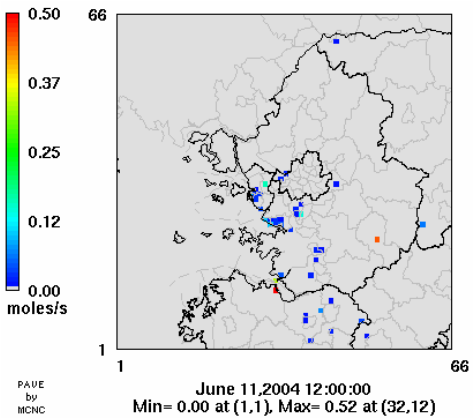


Figure 4.2 Spatial distributions of the CAPSS NO emissions processed by SMOKE for a 3-km resolution domain. For point sources, the emissions rates are shown for the surface layer only.

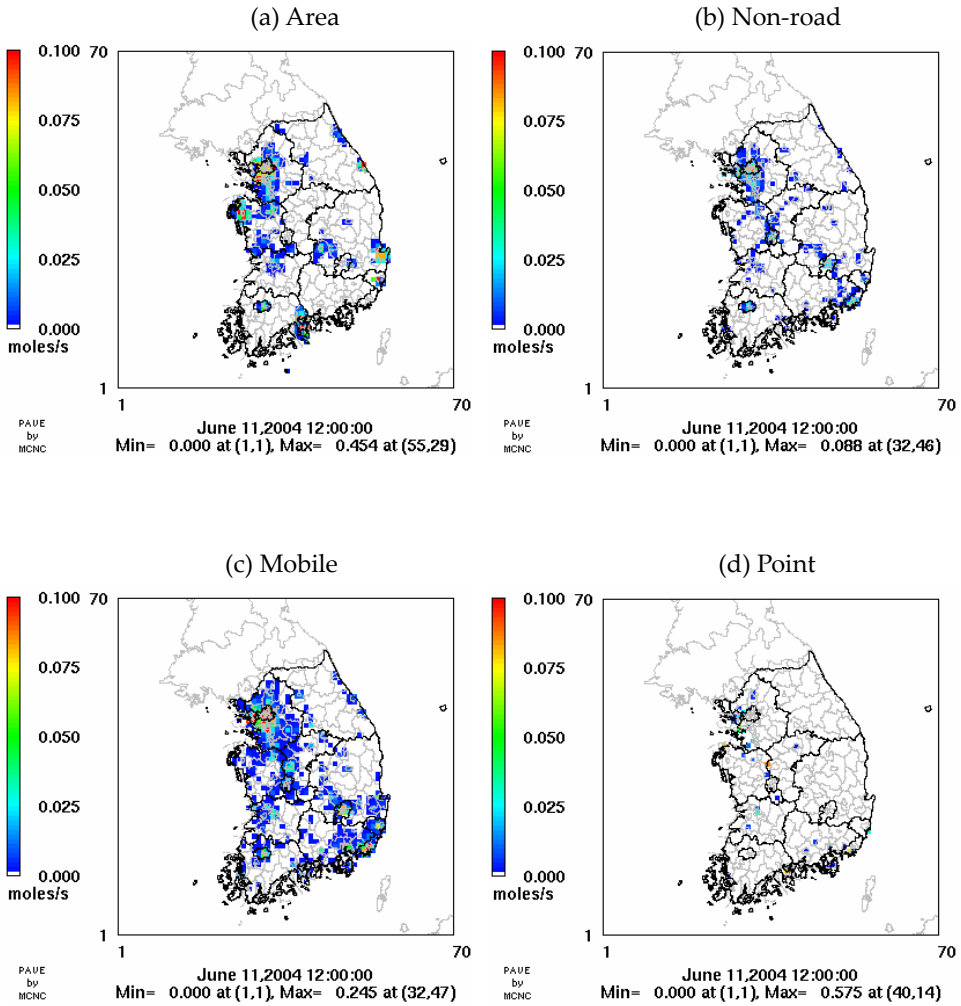


Figure 4.3 Spatial distributions of the CAPSS ETH emissions processed by SMOKE for a 9-km resolution domain. For point sources, the emissions rates are shown for the surface layer only.

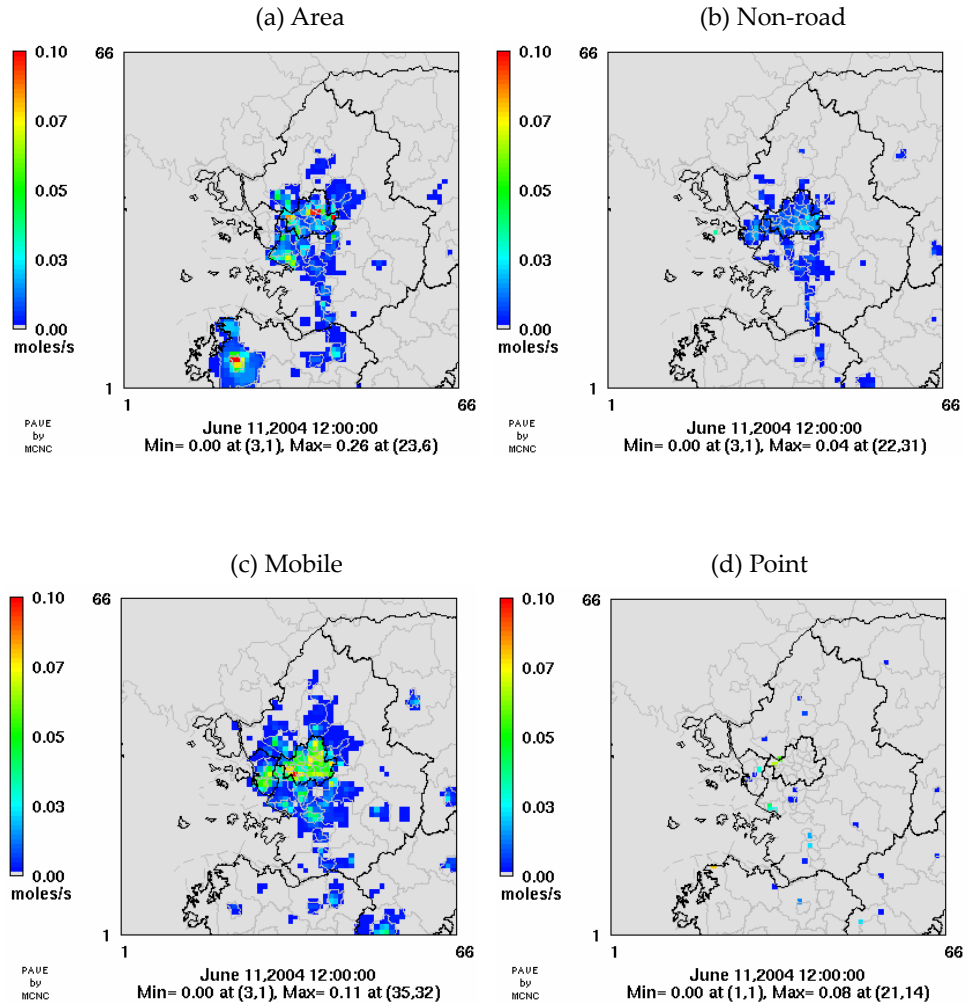


Figure 4.4 Spatial distributions of the CAPSS ETH emissions processed by SMOKE for a 3-km resolution domain. For point sources, the emissions rates are shown for the surface layer only.

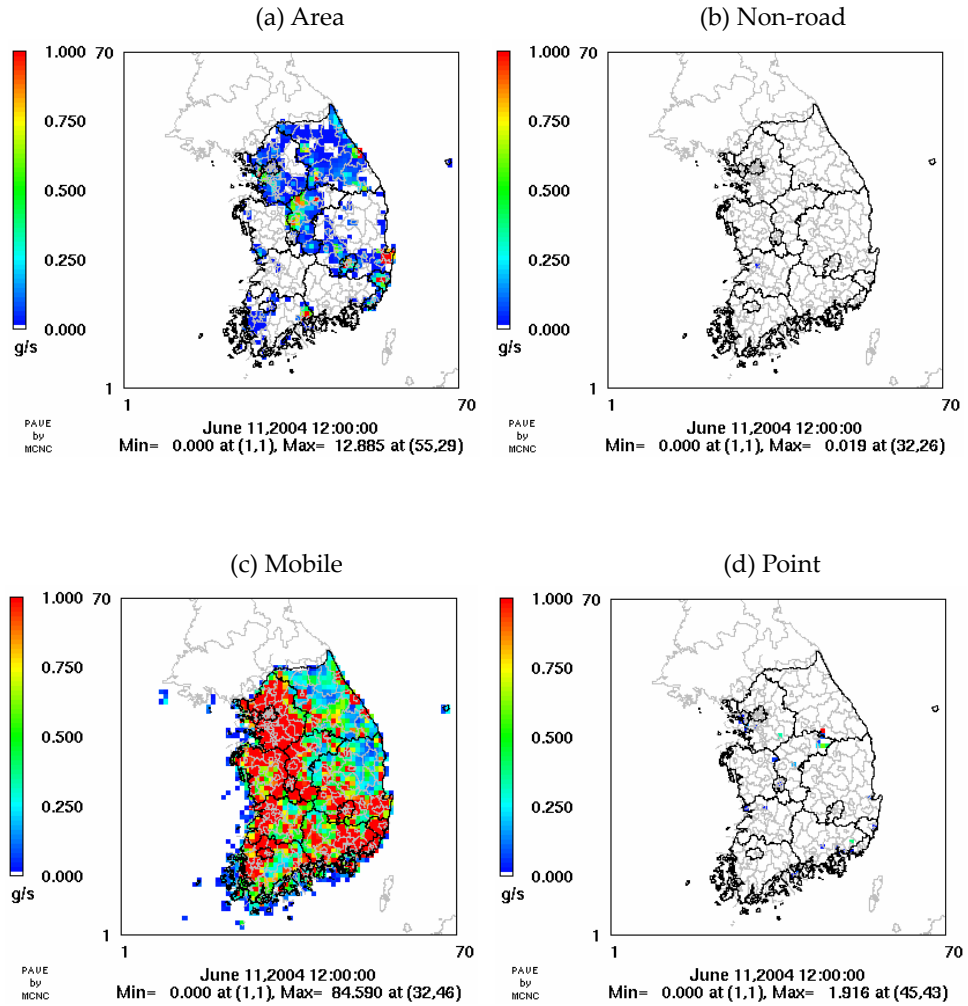


Figure 4.5 Spatial distributions of the CAPSS PMFINE emissions processed by SMOKE for a 9-km resolution domain. For point sources, the emissions rates are shown for the surface layer only.

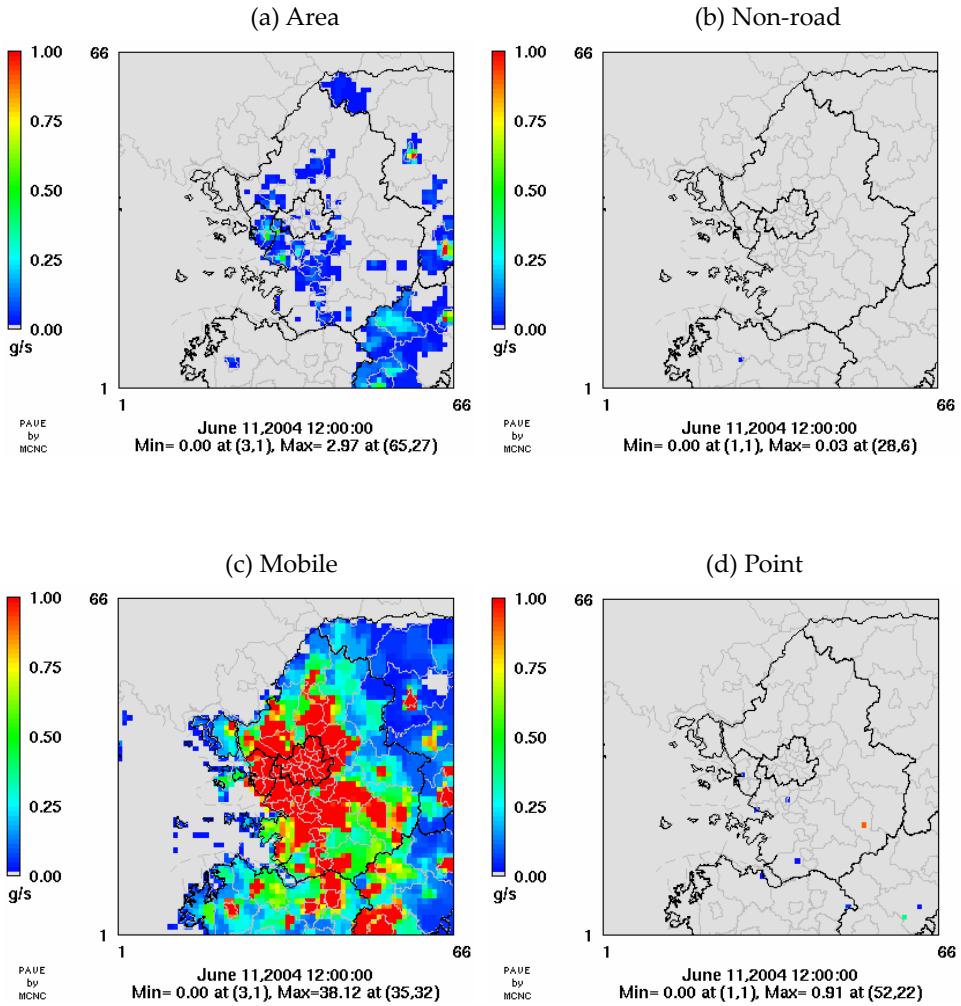


Figure 4.6 Spatial distributions of the CAPSS PMFINE emissions processed by SMOKE for a 3-km domain. For point sources, the emissions rates are shown for the surface layer only.

2. Chemical Speciation

The most popular atmospheric chemistry mechanisms used in comprehensive air quality models are the Carbon Bond 4 (CB4) chemical mechanism and the SAPRC99 chemical mechanism. These mechanisms are hybrids of explicit chemistry, surrogate approximations, and, lumped or generalized chemistry designed to simulate urban smog chemistry. Explicit chemistry is used for the inorganic species in both chemical mechanisms.

These mechanisms use distinctively different representations of the organic chemistry. Some organic species, which react slower or faster than other members of a group, are represented explicitly. CB4 includes explicit VOC species such as formaldehyde, ethylene, and isoprene. In SAPRC99, besides those species, there are more organic compounds represented explicitly, for example methane, acetaldehyde, acetone, methanol, and glyoxal. The CB4 mechanism employs different lumping techniques from the SAPRC99 mechanism for the remaining organic species. The CB4 mechanism relies on the lumped structure approach that uses carbon bond surrogates to represent most of the organic species, and the lumped molecule approach to represent aromatic species. The SAPRC99 mechanism uses either the lumped molecule approach (the same class of species lumped together) or the variable lumped parameter approach (lumping based on the reactivity of species). The complex mixture of urban hydrocarbons (hundreds of species routinely identified) is represented by only 18 CB4 modeled species and over 50 in the case of SAPRC99.

By implementing the CAPSS into SMOKE, it becomes possible to process the emissions inventory for any chemical mechanisms such as CB4, SAPRC99 , and RADM2 without additional works. For example, the SAPRC99 chemical mechanism can be used for chemical speciation, and the outputs were simulated with CMAQ to compare and to see the differences in the CB4 and SAPRC99 mechanisms. Table 4.1 shows available species after chemical speciation for CB4 and SAPRC99 mechanisms.

In order to simulate ambient PM concentrations, the precursors such as SO_2, NH_3 and VOC as well as PM should be prepared for model inputs. PM10 and TSP emissions are available form the CAPSS, but it does not include

PM2.5 emissions which is required for aerosol simulations. At this moment, it is roughly assumed that a 50% of PM10 explains PM2.5 emissions and added to SMOKE-ready emissions files during the data format conversion. A new PM2.5 inventory must be collected to remedy this problem. Once PM2.5 is inputted to SMOKE, it becomes speciated into PEC, POA, PNO3, PSO4, and PMFINE.

The chemical speciation results with the CAPSS emissions inventory for the CB4 chemical mechanism is explained with temporal variation in the next section.

Table 4.1 Chemical species for CB4 and SAPRC99 mechanisms.

Species in EI		Species after chemical speciation		Remarks
		CB4	SAPRC99	
Gas phase pollutants	CO	CO		
	NOx	NO NO_2		

	VOC	ALD2 ETH FORM ISOP NR OLE PAR TOL XYL	ACET ALK1 ALK2 ALK3 ALK4 ALK5 ARO1 ARO2 BALD CCHO CCO_OH CH4 CRES ETHENE GLY HCHO	HCOOH IPROD ISOPRENE MACR MEK MEOH MGLY NR OLE1 OLE2 PHEN PROD2 RCHO RCO_OH TRP1	Using 'TOC' profile

Table 4.2 Emissions species for aerosol modeling in SMOKE processing.

Species in EI		Species after chemical speciation		Remarks
		CB4	SAPRC99	
Gas	NH_3	NH_3		
	SO_2	SO_2 SULF	SO_2 X	
Particulate matters	PM10	X (Skipping)	PM10(Unit conversion)	
	PM2.5	PEC PMFINE PNO3 POA PSO4	PEC PM2.5 PMFINE PNO3 POA PSO4	
	PMC	PMC	PMC	PMC=PM10 – PM2.5

3. Temporal Allocation

Figure 4.7 presents temporal variations of domain-wide NO, CO, PAR, ETH, and OLE emissions for the 9-km resolution domain which covers the whole area of South Korea and therefore includes all the emissions in the CAPSS emissions inventory. June 12th, 2000 was a Saturday and on-road mobile emissions on that day showed slightly different diurnal variations than those for weekdays. Emissions rates from non-road and area sources present sinusoidal diurnal variations, showing the highest peak during daytime when activity levels reach the peaks.

For the South Korean domain, on-road mobile sources take ~ 50 % of NO emissions during daytime, showing morning and evening peaks, followed by point, non-road, and area sources. Compared to other sources, emissions rates for point sources show small diurnal variations due to the continuous operation patterns assumed.

CO emissions rates are mostly explained by mobile sources and the contributions from other sources become negligible. It is seen that the nation-wide CO emissions is heavily dependent on mobile sources in the CAPSS emissions inventory.

After chemical speciation of lumped VOC emissions, PAR emissions from area sources are higher than those from other sources, increasing in the morning and decreasing in the evening. It is also shown that PAR emissions from on-road mobile sources increase during daytime, while PAR emissions from non-road mobile sources are insignificant.

ETH and OLE are more reactive species in the CB4 chemical mechanism. For ETH emissions, point sources show higher contribution than other sources. It is noticeable that on-road mobile and area sources become important during daytime with increased ETH emissions compared to nighttime. For OLE emissions, on-road mobile sources become the dominant sources followed by point and area sources.

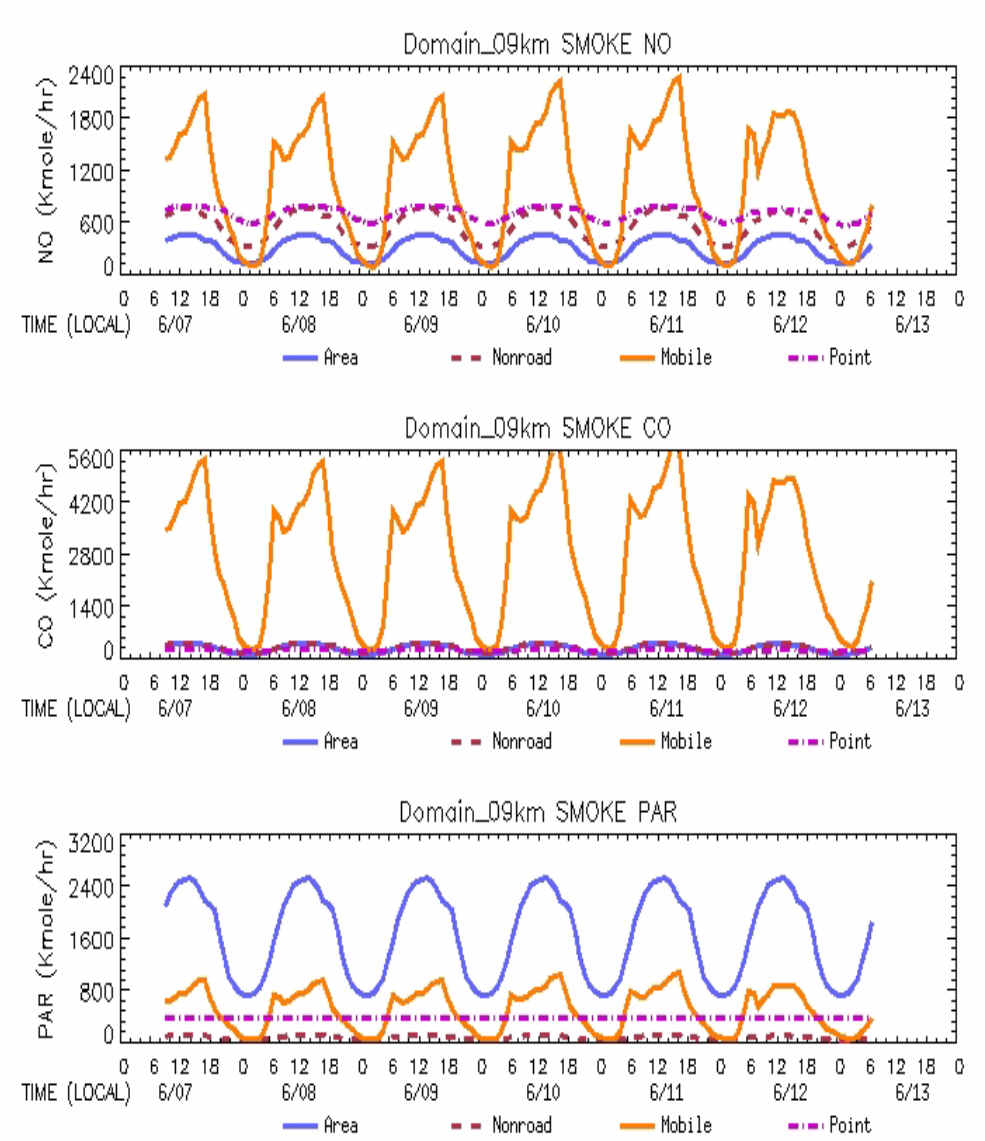


Figure 4.7 Temporal variations of (a) NO, (b) CO, (c) PAR, (d) ETH, and (e) OLE emissions for a 9-km resolution domain.

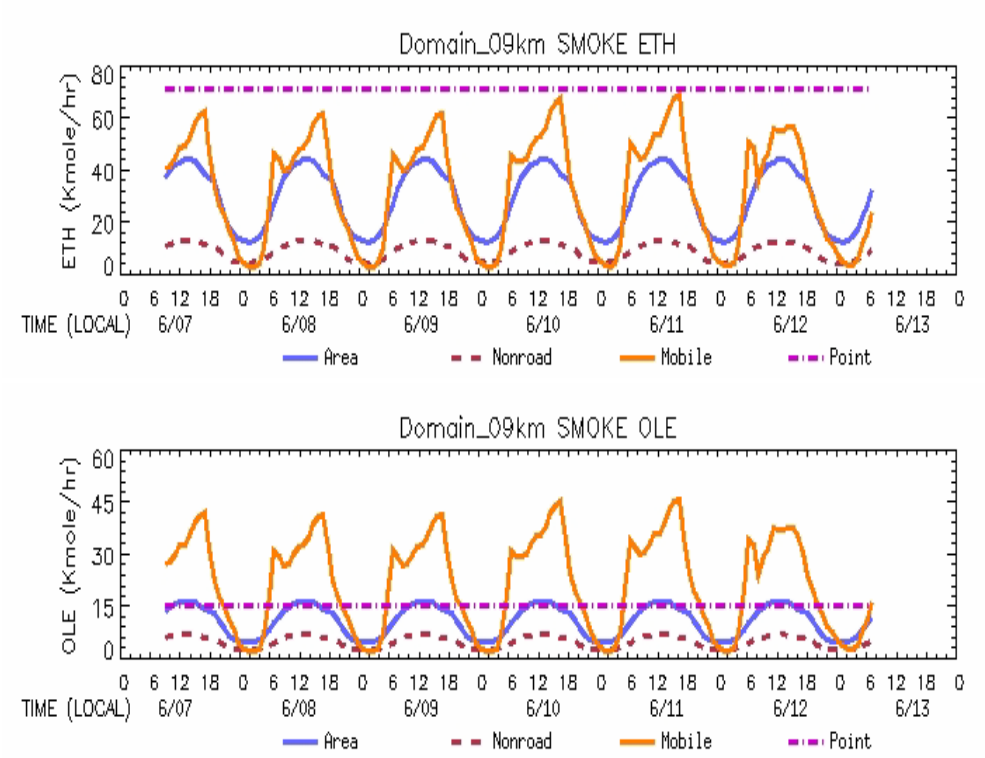


Figure 4.7 Continued.

Temporal variations of domain-wide NO, CO, PAR, ETH, and OLE emissions for the 3-km resolution domain were presented in Figure 4.8. The domain covers Seoul, Incheon, Gyeonggi-do, and neighboring regions in part.

For the 3-km resolution domain, NO emissions are mostly contributed by on-road mobile sources and followed by non-road mobile, point, and area sources. Similar to the 9-km resolution domain, CO emissions rates here are mostly coming from on-road mobile sources, and other sources become negligible for the emissions in the emissions inventory.

For PAR emissions, area sources are the dominant sources, but point sources becomes insignificant for the 3-km resolution domain with less numbers of sources, decreased amounts of VOC emissions, and different

source characteristics for chemical speciation.

For ETH emissions, on-road mobile sources show the highest emissions rates during daytime, while point sources present relatively high contribution persistently without diurnal variations. Area sources become important during daytime with the emissions rates increased.

For OLE emissions, on-road mobile sources are the dominant sources for the domain followed by area sources.

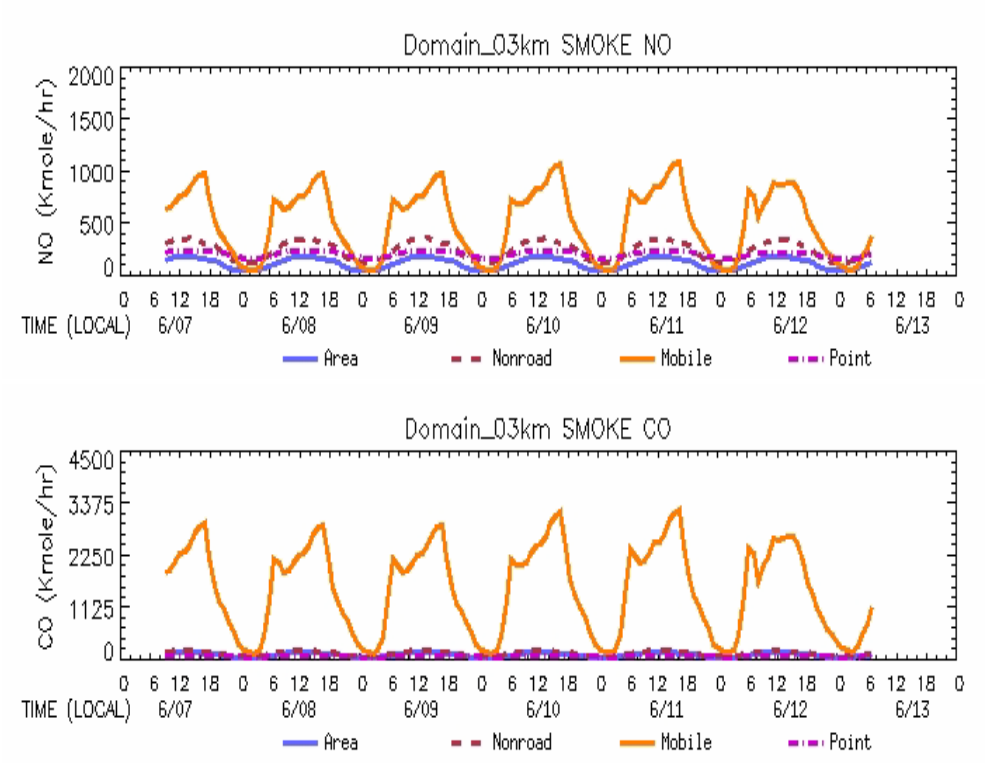


Figure 4.8 Temporal variations of (a) NO, (b) CO, (c) PAR, (d) ETH, and (e) OLE emissions for a 3-km resolution domain.

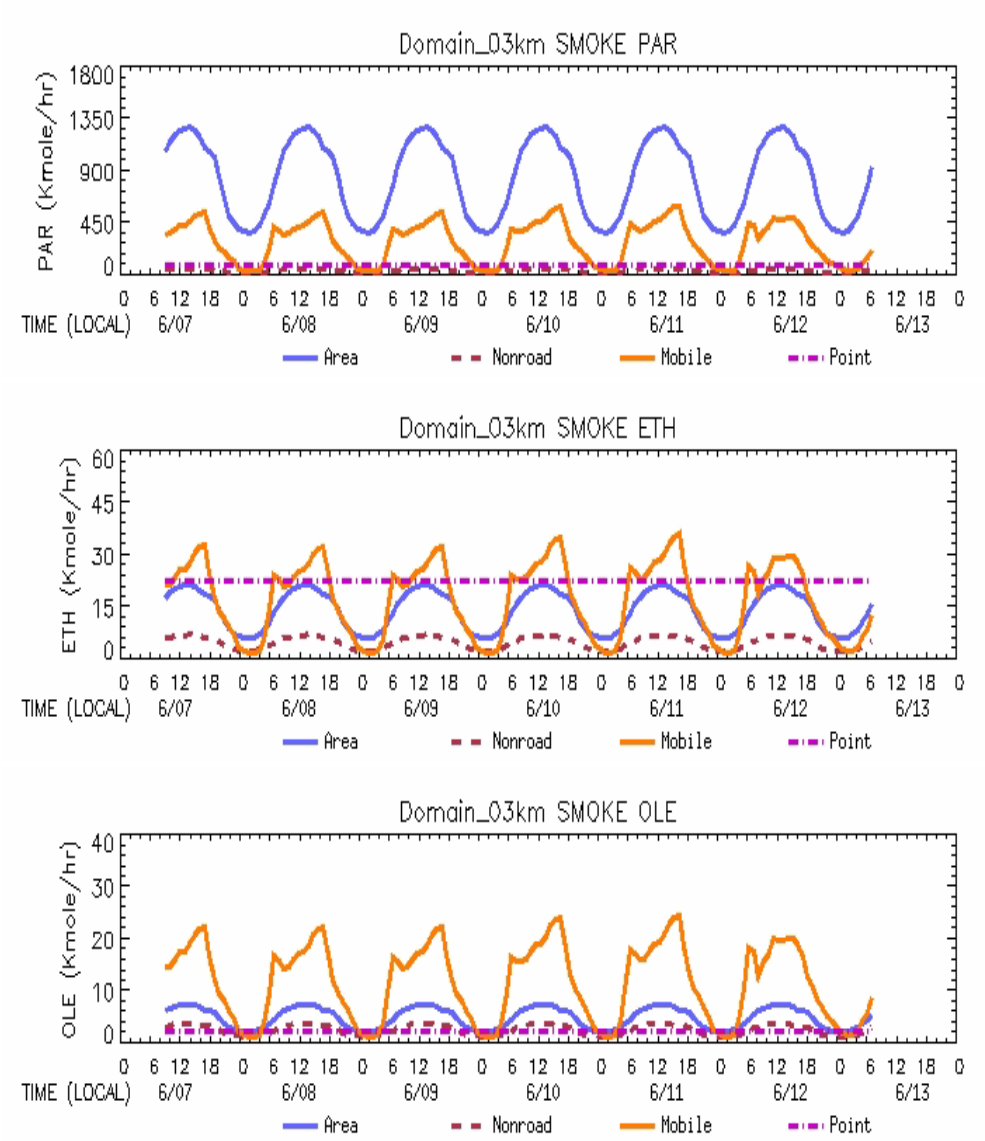


Figure 4.8 Continued.

4. Plume Rise of Point Source Emissions

With MM5-MCIP outputs describing hourly meteorological conditions, point source emissions are vertically allocated to generate fractional emission distribution in the vertical layers. The SMOKE plume-rise algorithms compute plume top and bottom heights based on stack parameters such as stack height and diameter, and exit temperature and velocity of an exhausting plume for given meteorological conditions. Once plume top and bottom heights are determined, the fractional portion of emissions rates for each species is estimated for each vertical layer, depending on a vertical structure setup.

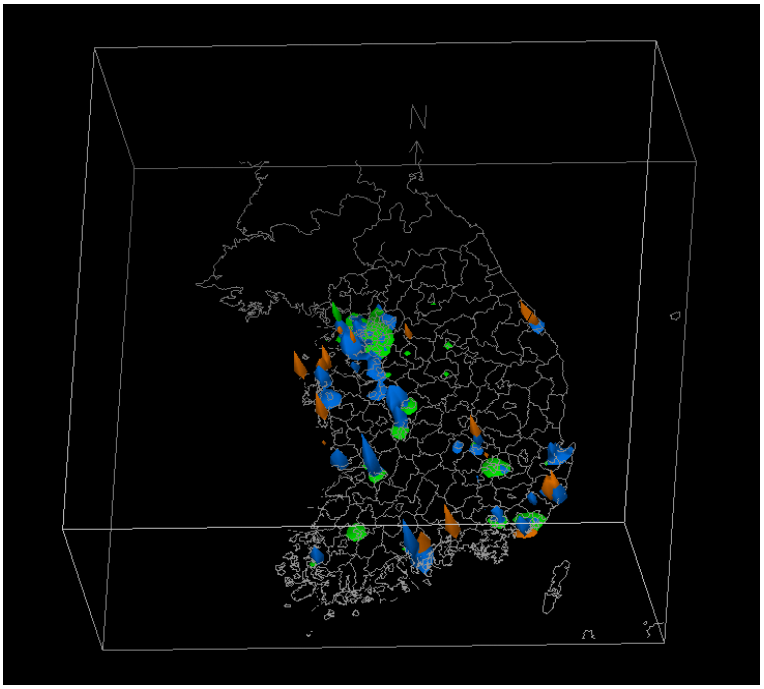


Figure 4.9 A top view of the CAPSS processed for a 9-km domain. CO, SO_2, and VOC emissions are represented with green, orange, and blue, respectively.

Figure 4.9 and 4.10 show iso-surface plots for several emissions species selected. As shown, emissions of the cells with large point sources are vertically distributed, and the top heights that emissions plumes reach vary from source to source. In Figure 4.9, NO emissions (green) from all the sources including area and mobile sources are also displayed. Cells over large cities, such as Seoul and Busan, show high NO emissions located at lower altitudes representing the emissions from mobile and area sources.

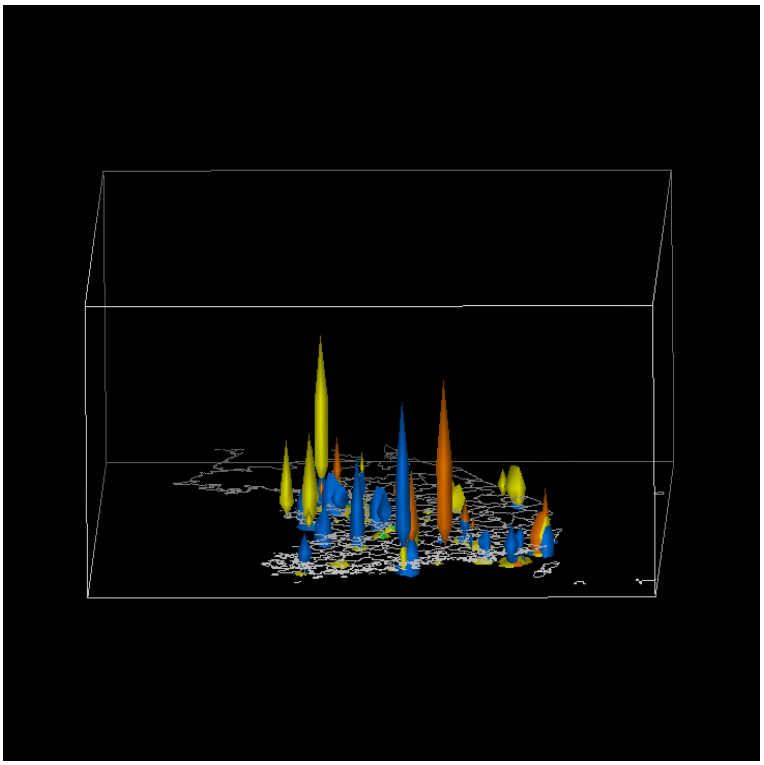


Figure 4.10 A south view of the CAPSS processed for a 9-km domain. CO, SO_2, and VOC emissions are represented with green, orange, and blue, respectively.

Chapter 5. Application of KEI-EIPS on Seoul Metropolitan Area Using CMAQ

1. CMAQ Overview

A set of preprocessors provides linkage mechanisms among the meteorology, emissions, and chemistry transport modeling components. These processors include: the Emission-Chemistry Interface Processor (ECIP) that translates data from the SMOKE emission model for use in the CCTM; the Plume Dynamics Model that computes geometry of sub-grid scale lagrangian plumes for large elevated emitters; and the Meteorology-Chemistry Interface Processor (MCIP) that translates and processes outputs from the meteorology model for the CCTM. Initial Conditions and Boundary Conditions (ICON and BCON) provide concentration fields for individual chemical species for the beginning of a simulation and for the grids surrounding the modeling domain, respectively. The ICON and BCON processors use data provided from previous three-dimensional model simulations or from clean-troposphere vertical profiles. Both the vertical profiles and modeled concentration fields have specific chemical mechanisms associated with them, which are a function of how these files were originally generated. And the photolysis processor (JPROC) calculates temporally various photolysis rates. MCIP interpolates the meteorological data if needed, converts between coordinate systems, computes cloud parameters, and computes surface and planetary boundary layer (PBL) parameters for the CCTM. MCIP uses land-use information from the land-use processor (LUPROC) to calculate the PBL and surface parameters.

The CCTM simulates the relevant and major atmospheric chemistry, transport and deposition processes involved throughout the modeling domains. The science options available to the user include the gas phase chemistry mechanisms, RADM2 and CB4, a set of numerical solvers for the mechanisms, options for horizontal and vertical advection schemes,

algorithms for fine and coarse particulate matter predictions, photolysis rates, and a plume-in-grid approach. Through the Models-3 framework, CMAQ simulations can be developed using these different options without modifying source code. The arrows in Figure 5.1 show the flow of data through the modeling system.

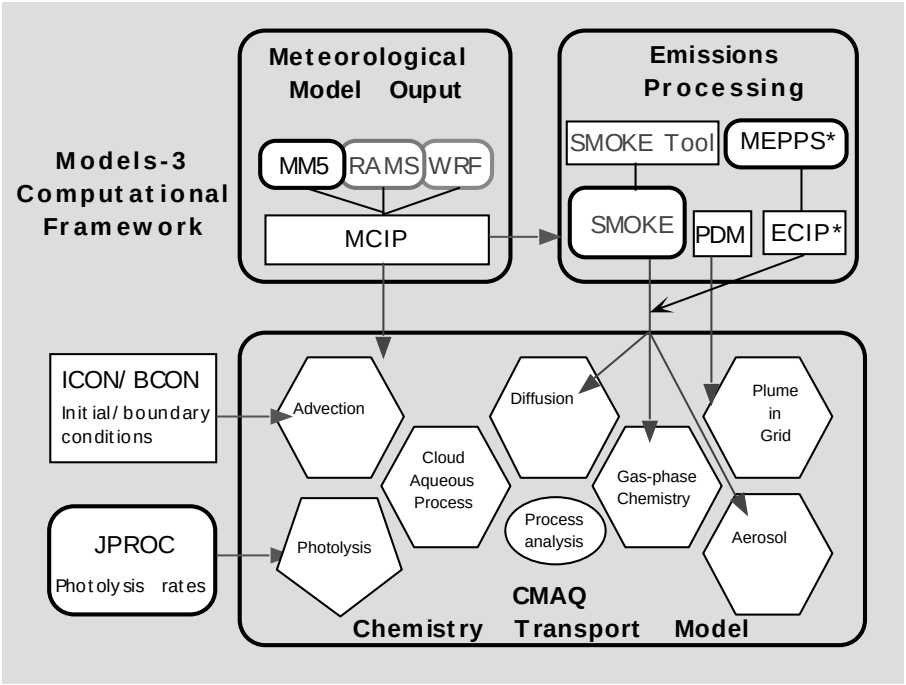


Figure 5.1 Emissions and Meteorological modeling systems and the CMAQ Chemical Transport Model and Interface Processor.

2. Configuration

To apply the KEI-EIPS system that was developed as an emissions preparation system capable of temporally and spatially allocating and chemically speciating the CAPSS emissions inventory for an air quality modeling application suitable for the user's approach. In addition to demonstrate the use of the air quality modeling and analysis infrastructure, air quality simulations and data analyses were performed over the Seoul Metropolitan area for 01 June – 15 June, 2004. The experiment period includes two high ozone spikes; 10 and 11 June. We have used the MM5 meso-scale meteorology model, SMOKE emissions processing systems, EPA's CMAQ air quality models for the simulations. As shown in Table 5.1, we have selected CB4 chemical mechanism with EBI(Euler Backward Iterative) solver in CMAQ simulations.

Table 5.1 CMAQ Simulation Configuration.

Model Configuration	
Meteorology Data	MM5/NCAR-Penn State Univ.
Emission	CAPSS 2003
Chemical Mechanism	CB4
Simulation Domain	27km - 9km - 3 km
Simulation Period	01 June ~ 15 June, 2004

3. Comparison of CMAQ Results to the Observation

Emissions tuning can be exercised to have more comparable simulation results to the observations for a given condition. It was, however, aimed in this study to evaluate the KEI-EIPS system by appling with the CAPSS data to prepare input data to an air quality model.

Figures 5.2 ~ 5.5 show the time series of CMAQ-predicted O_3, NO_2, and CO concentrations compared to the surface observations for 5 ~ 15 June, 2004. There were two O_3 peak days during the evaluation period; 10 and 11 June, 2004, on which high O_3 concentrtions were observed over the Seoul Metropolitan area.

NO measurements were not available for all the observation sites, and the time series was not presented for those sites. After CMAQ simulations, predicted O_3 concentrations were well matched to those observed at Seosan Dongmoon-Dong and Seoul Yongdu-Dong sites. However, model simulations with the emissions inventory under-predicted O_3 concentrations over Seoul Bulgwang-Dong and Incheon Guwol-Dong sites. For the hours when O_3 under-predictions appeared, uncertainties in NO and NO_2 which would be over-estimates of those species were detected at the same time.

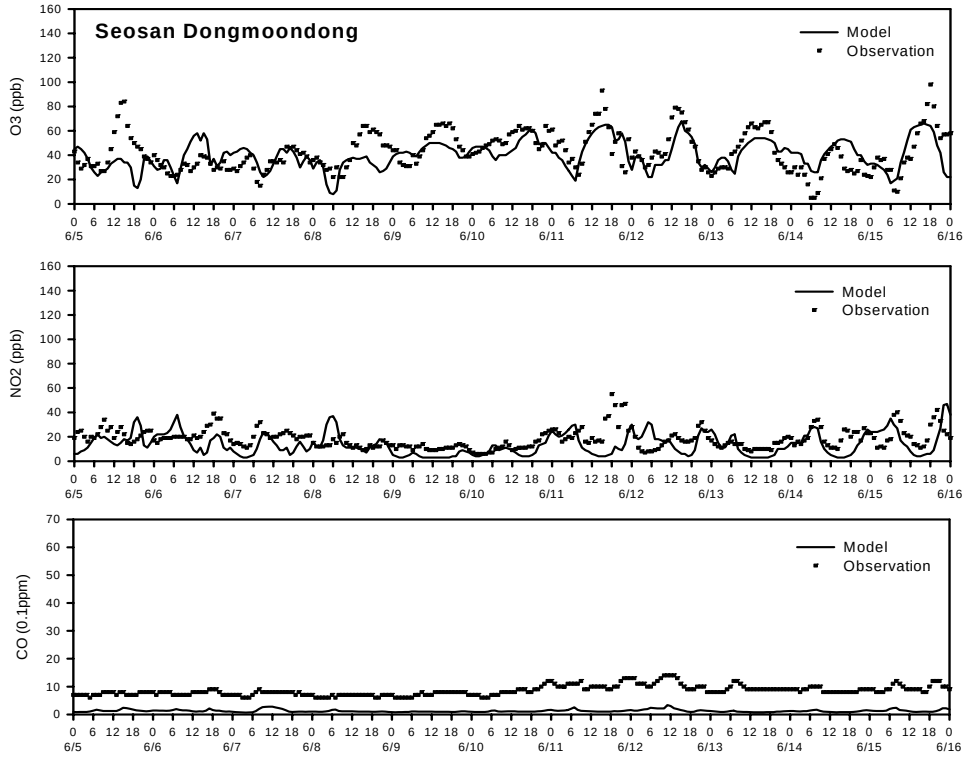


Figure 5.2 Simulated and observed time series of O_3, NO_2, NO and CO for surface station as the results of CMAQ(3km) for 5 ~ 15 June, 2004 at Seosan Dongmoon-Dong.

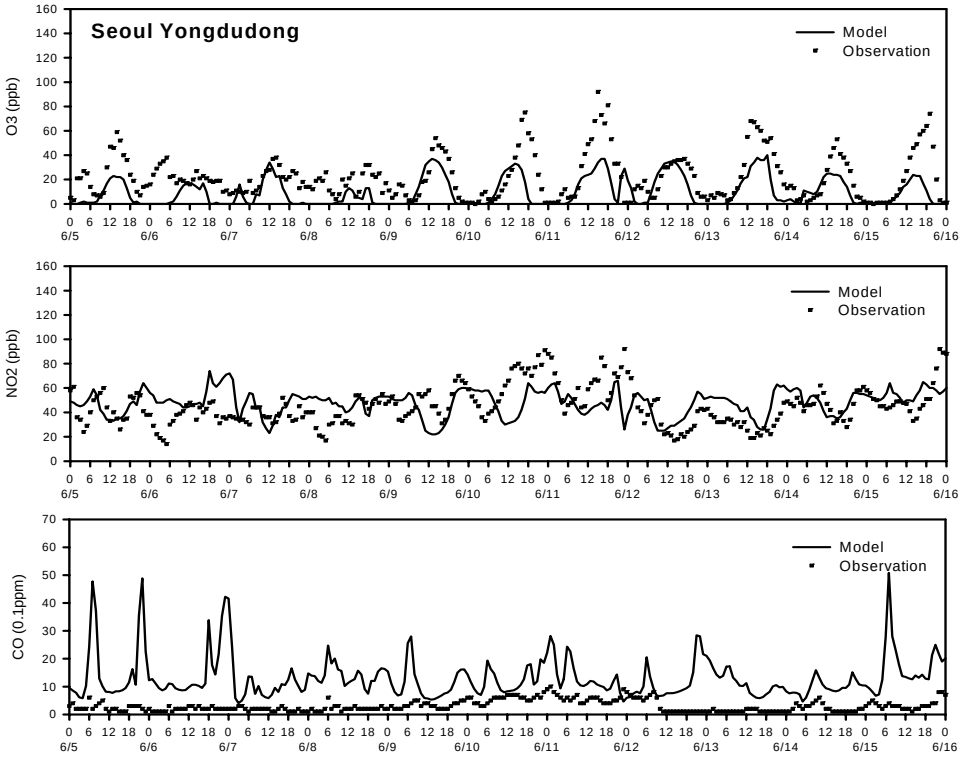


Figure 5.3 The same as Figure 5.2 except for Seoul Yongdu-Dong.

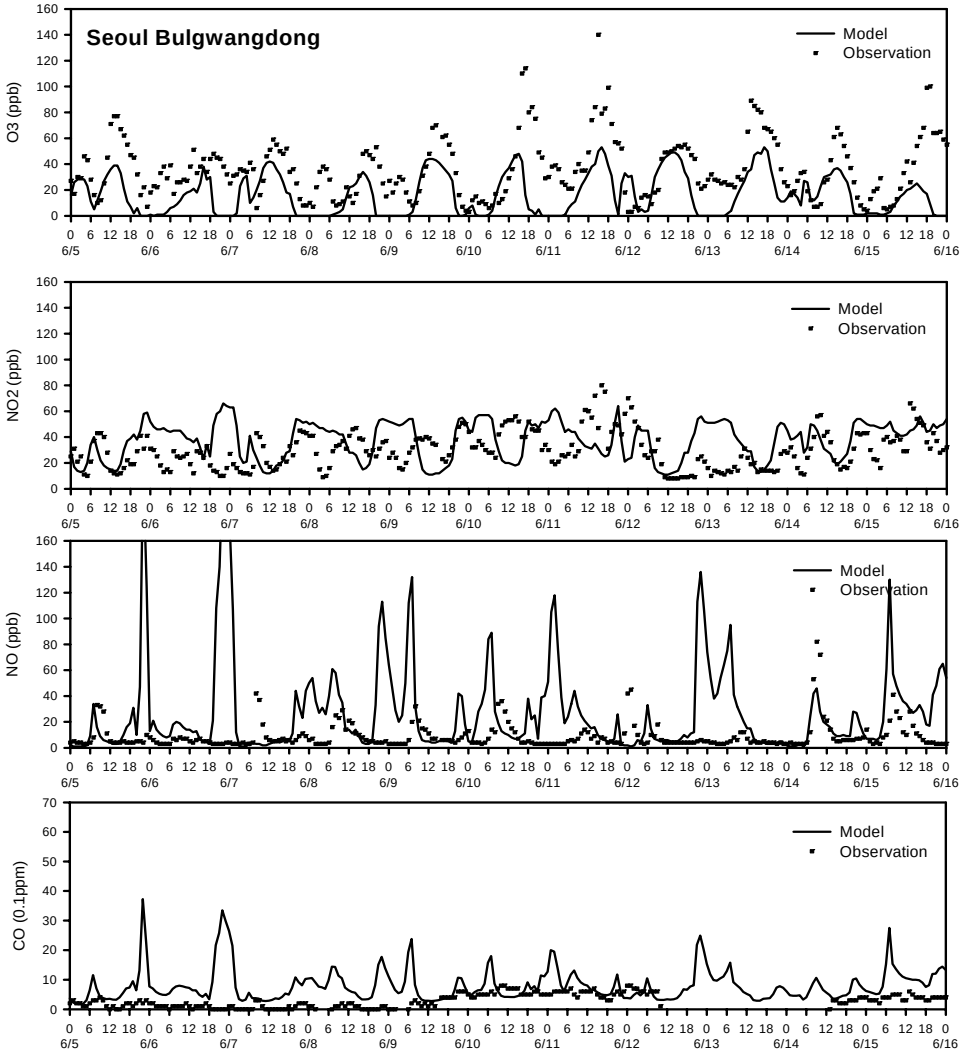


Figure 5.4 The same as Figure 5.2 except for Seoul Bulgwang-Dong.

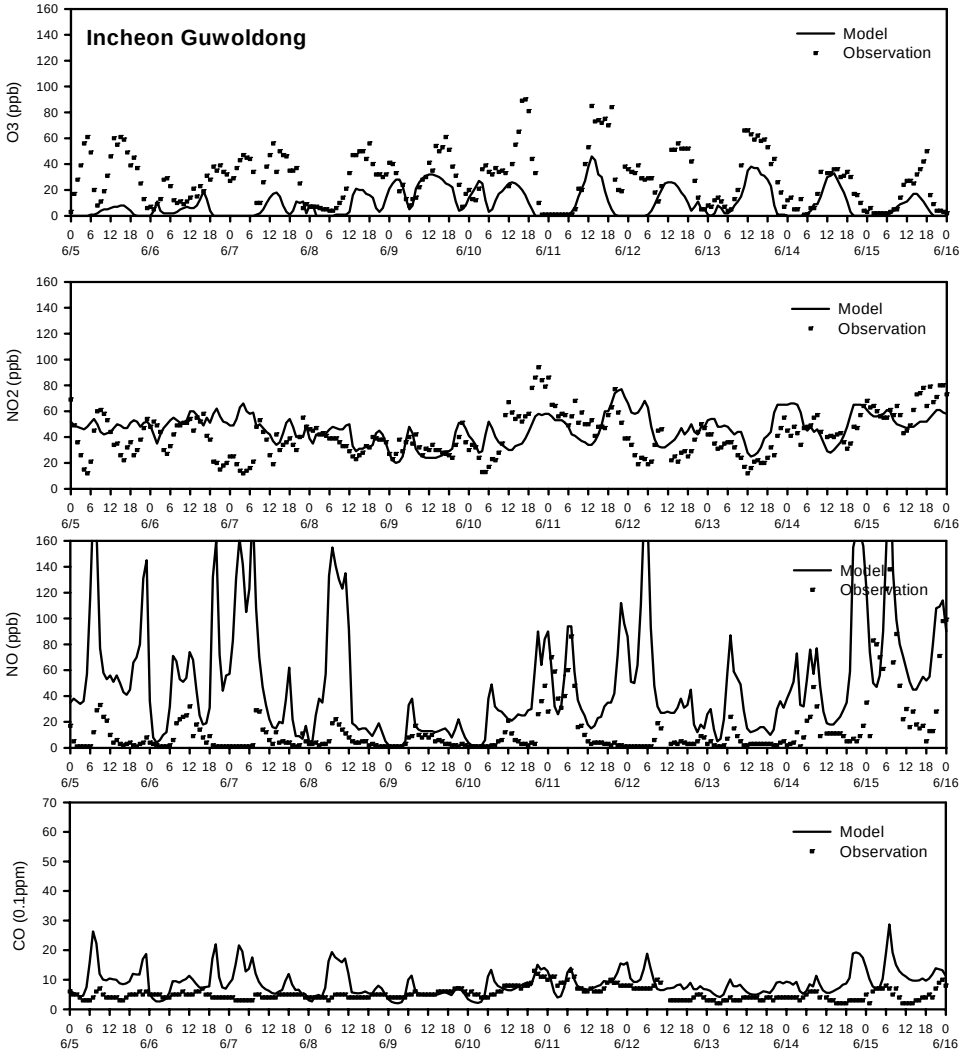


Figure 5.5 The same as Figure 5.2 except for Incheon Guwol-Dong.

Figure 5.6 ~ 5.9 present hourly varations of ETH, TOL, XYL and ISOP concentrations for 5 ~ 15 June, 2004. CMAQ results were compared to ETH, TOL, XYL and ISOP concentrations observed by Photochemical Assessment Monitoring Stations (PAMS). In order to evaluate the KEI-EIPS system for chemical speciation of lumped VOC emissions in CAPSS, it is necessary to compare model simulation results to the observations for VOC as well as other criteria species. PAMS measurements are mostly available chemicals speciated based on carbon bonds such as alkanes and alkenes, and it is needed to re-lump them to compare a model VOC speceis for a chemical mechanism selected. So explicitly comparable species such ETH, TOL, XYL and ISOP were evaluated in this study. In case of ETH and XYL, the prediction values are higer than PAMS values at Seoul Bulgwang-Dong and Incheon Guwol-Dong sites located in an urban area. On the other hand, Gwangju Tanbeol-Dong presents quite good results for the comparison between prediction and PAMS values of ETH and XYL. The ISOP values of CMAQ results show quite well matched with PAMS over most sites except for Ganghwa Seokmori. Ganghwa Seokmori is located in a sub-urban or rural area, so that high ISOP concentration was observed by PAMS, however CMAQ results do not show the magnitute of PAMS.

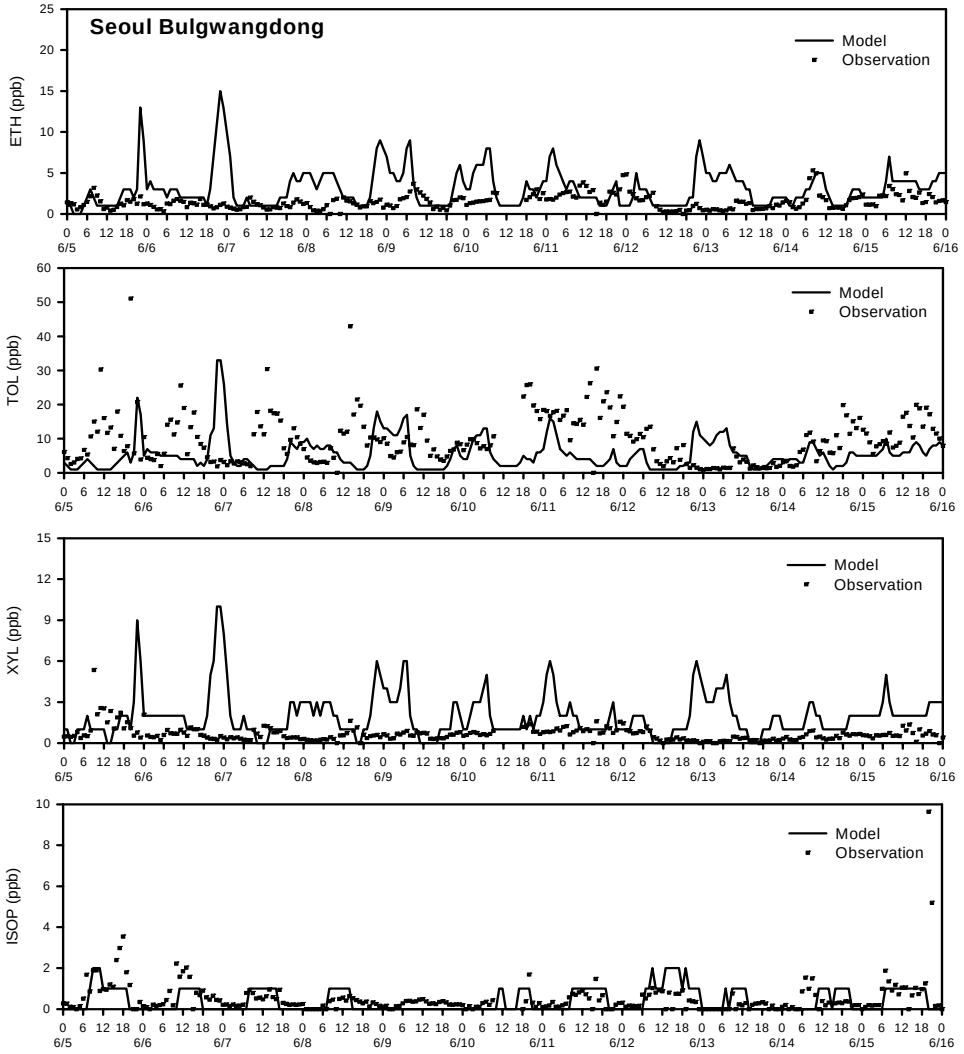


Figure 5.6 Simulated and observed time series of ETH, TOL, XYL and ISOP for surface station as the results of CMAQ(3km) for 5 ~ 15 June, 2004 at Seoul Bulgwang-Dong.

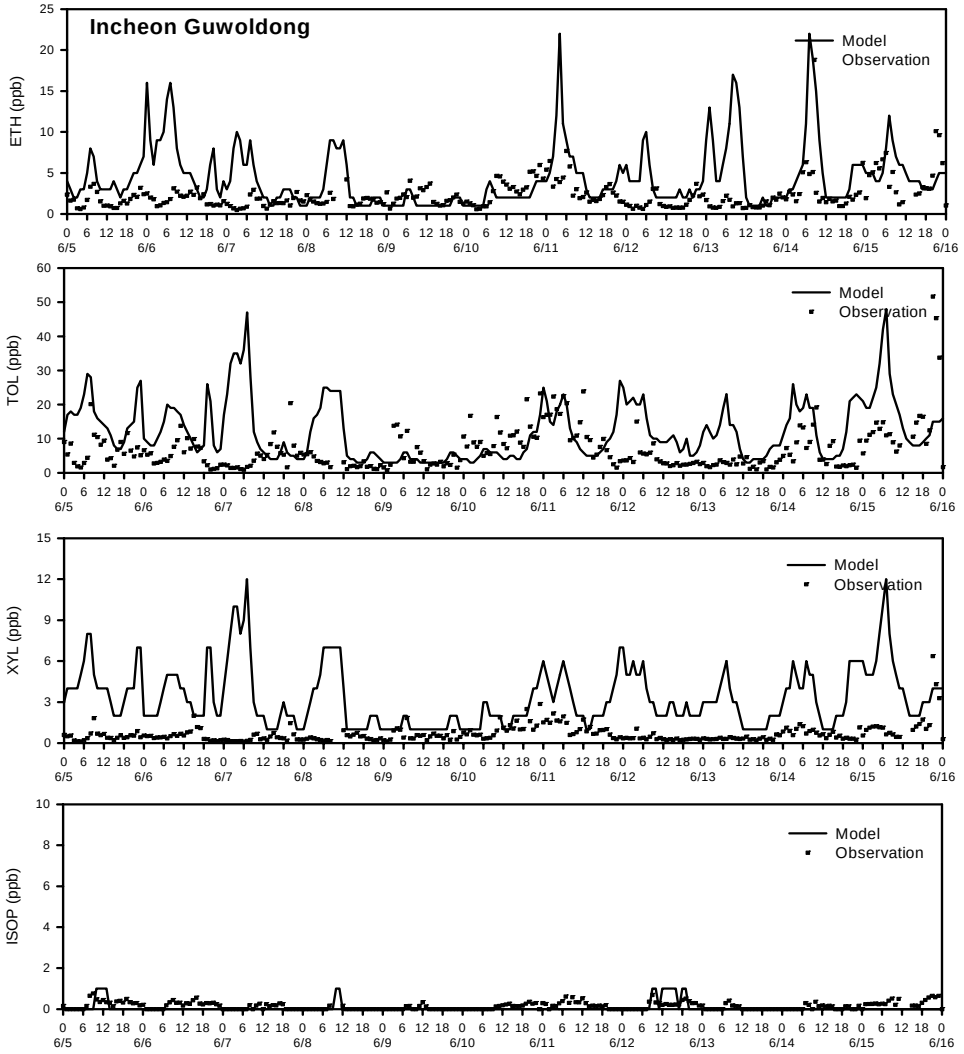


Figure 5.7 The same as Figure 5.6 except for Incheon Guwol-Dong.

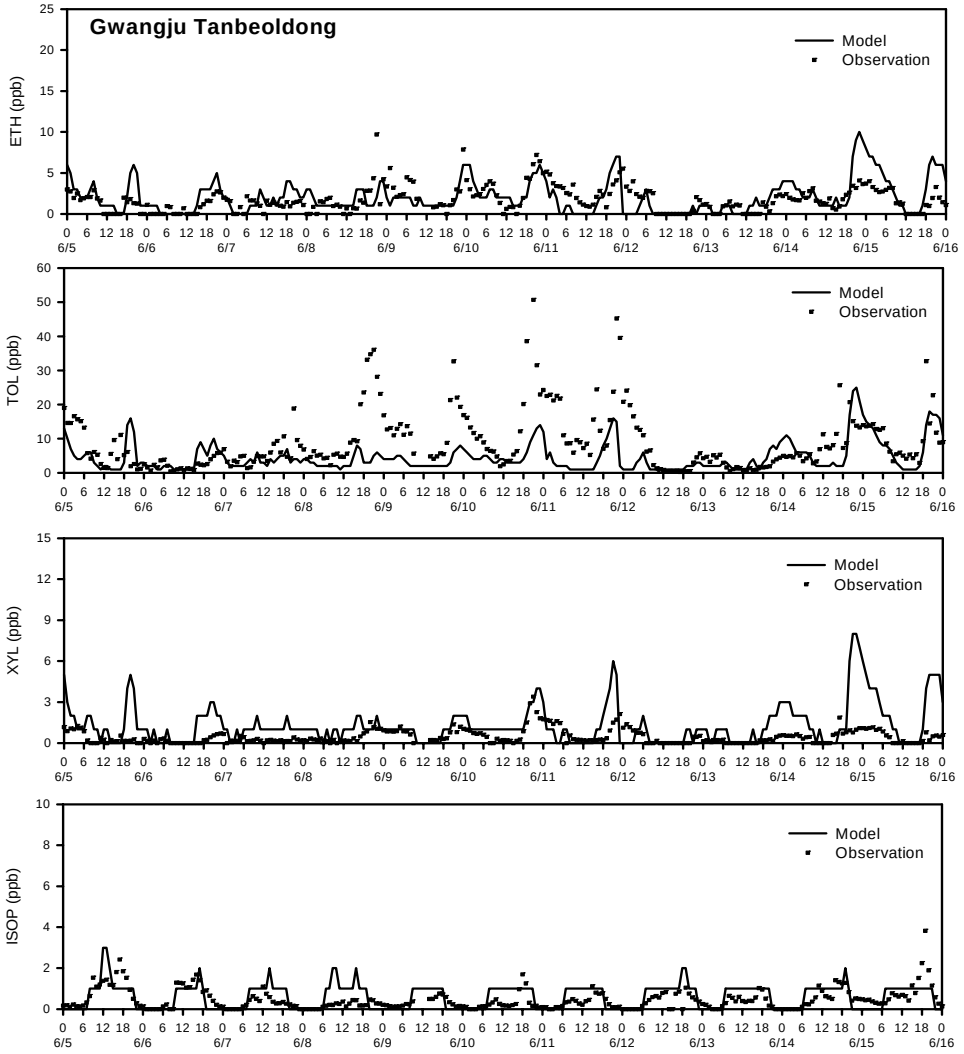


Figure 5.8 The same as Figure 5.6 except for Gwangju Tanbeol-Dong.

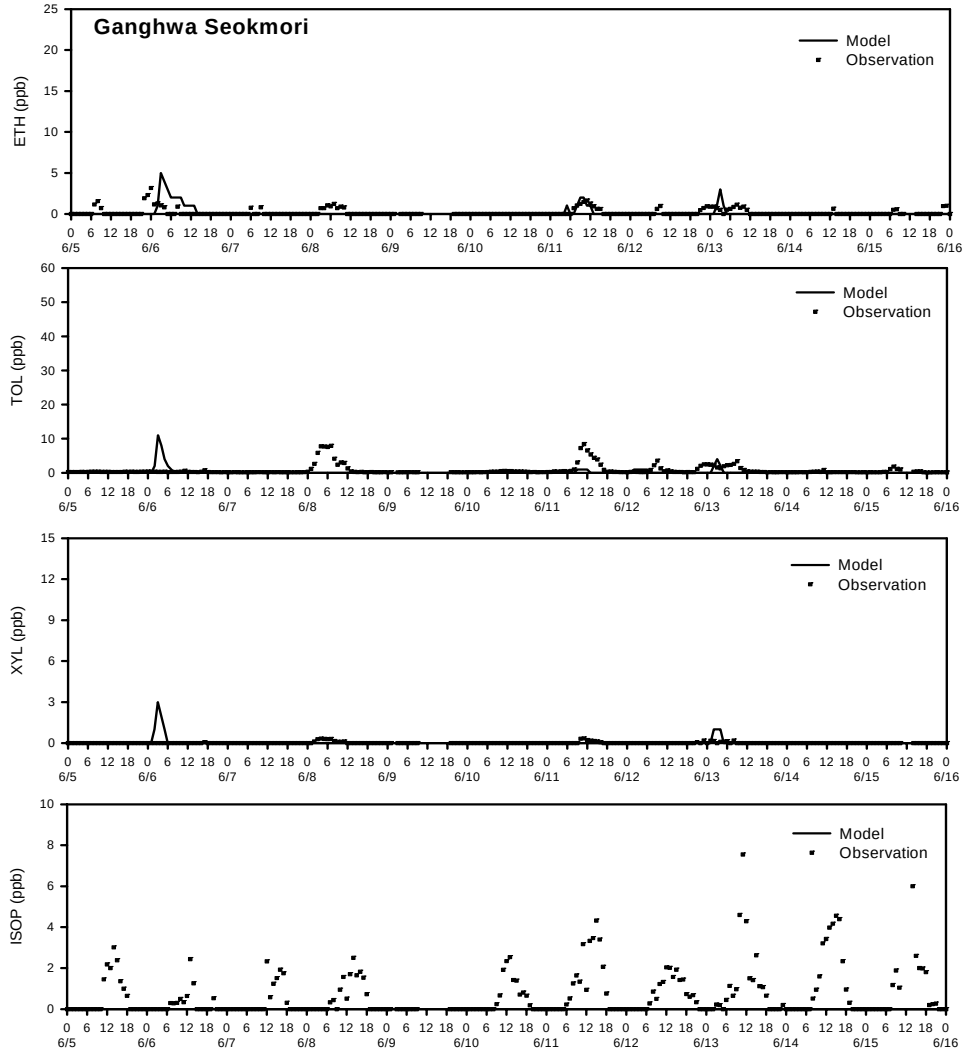


Figure 5.9 The same as Figure 5.6 except for Ganghwa Seokmori.

Figures 5.10 ~ 5.13 present horizontal distributions of wind vector and the simulated O_3, NO, NO_2, and CO concentrations on 11 June, 2004. As shown in those Figures, the area of low O_3 concentration is the same area as the high NO and NO_2 concentration over all time, especially on 03LST and 21LST. The overestimation of NO_2 and NO emission rate is related to the conduct of low O_3 production.

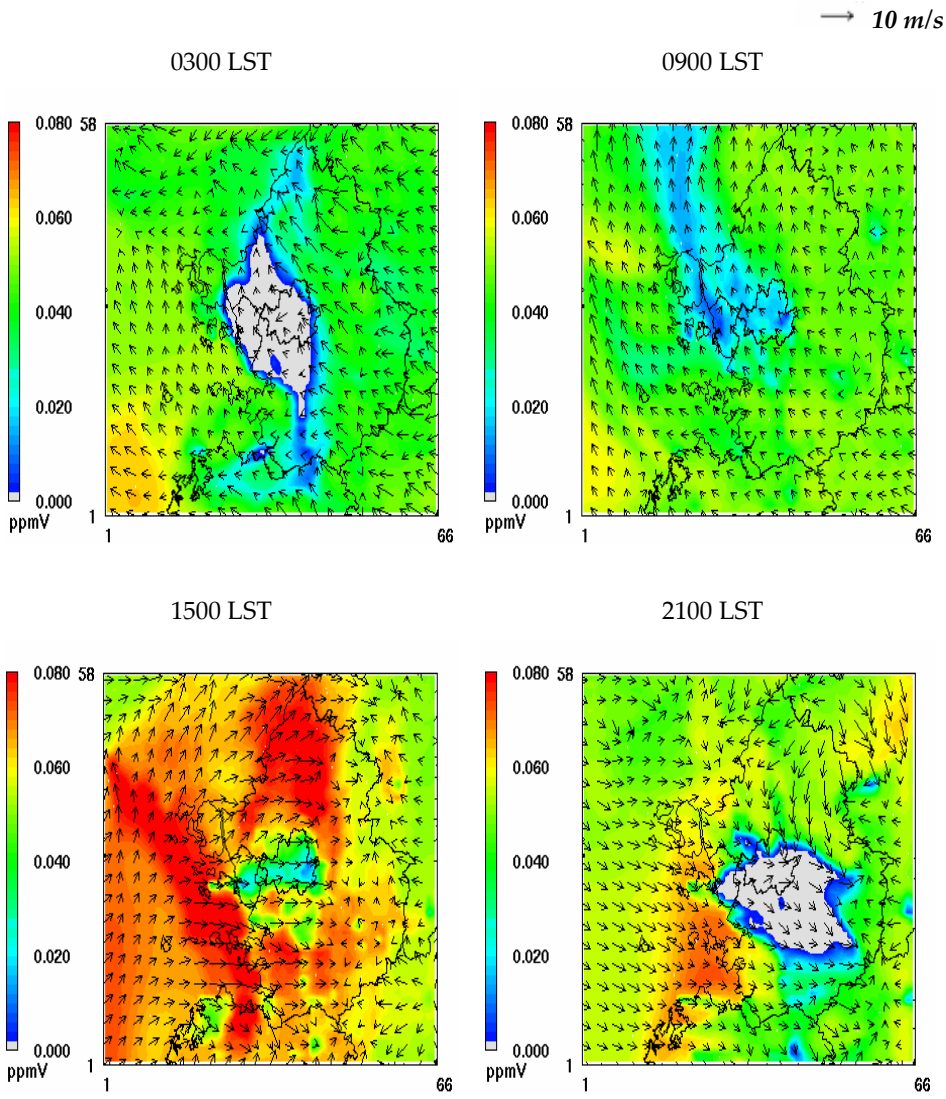


Figure 5.10 The horizontal distributions of wind vector and the simulated O_3 on 11 June, 2004.

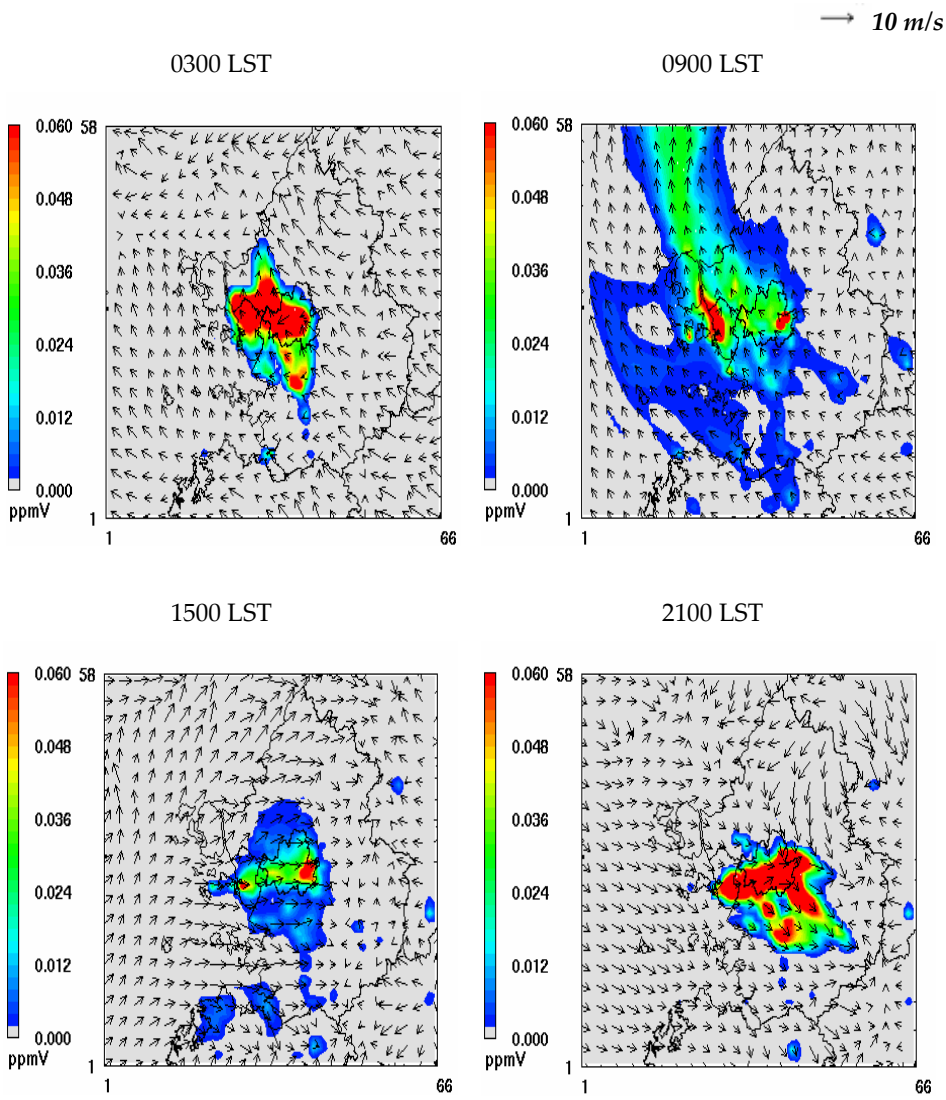


Figure 5.11 The horizontal distributions of wind vector and the simulated NO on 11 June, 2004.

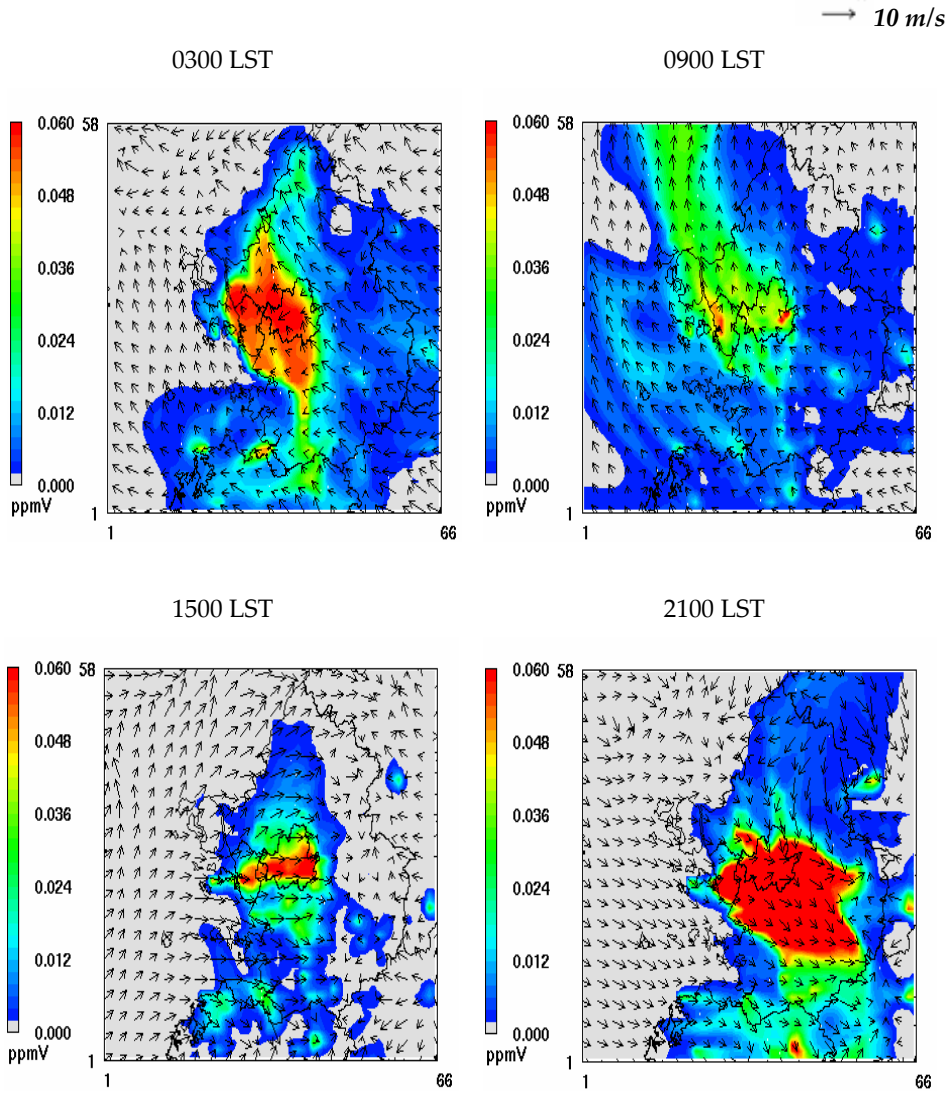


Figure 5.12 The horizontal distributions of wind vector and the simulated NO_2 on 11 June, 2004.

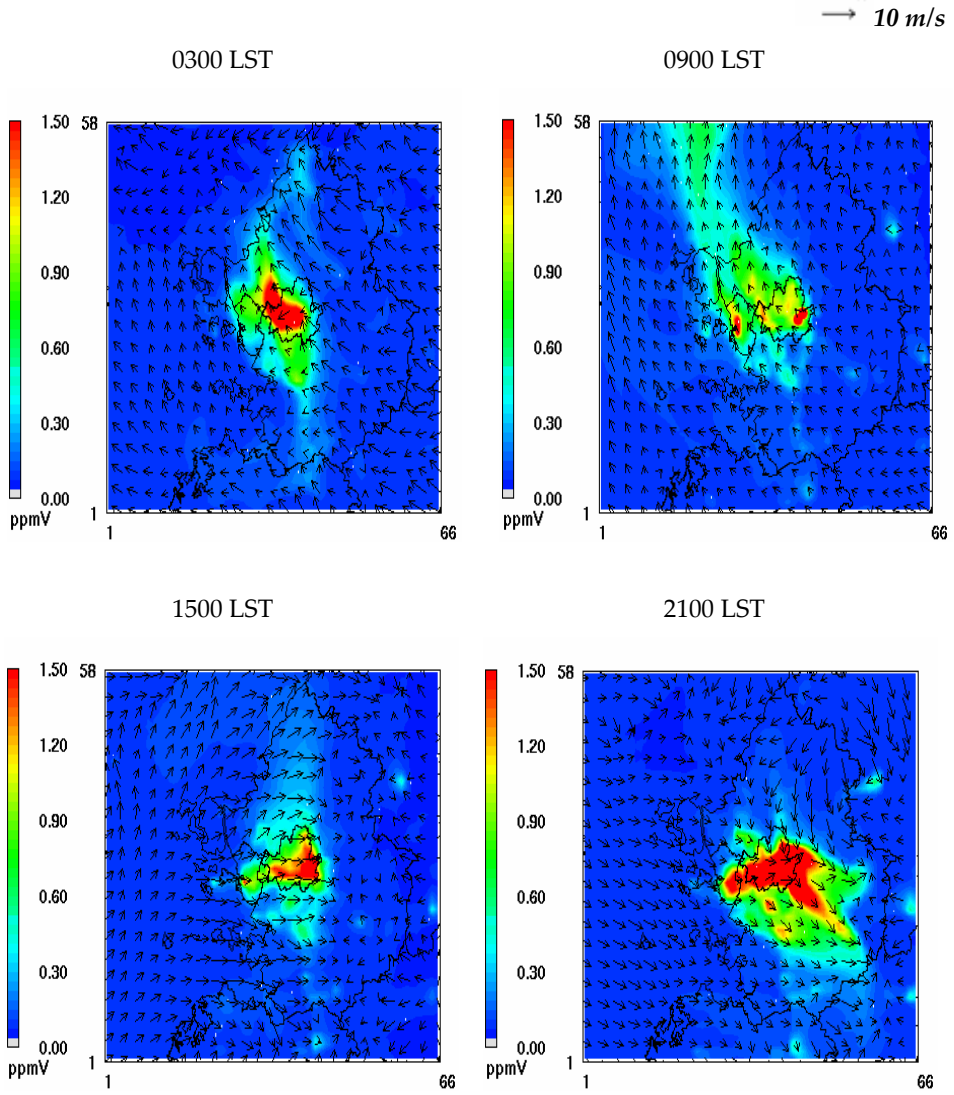


Figure 5.13 The horizontal distributions of wind vector and the simulated CO on 11 June, 2004.

Chapter 6. SMOKE Reports on the Emissions Inventory

Compared to other emissions processing systems, one of advantages we can take from the SMOKE system is its reporting function to summarize the emissions inventory processed. For example, it reports how much emissions for inventory species are generated from a region and from a source type.

Figure 6.1 represents NOx, VOC, CO, PM10, SOx, and NH_3 emissions from each source for each region. Annual emissions rates were used for area and mobile sources, while monthly emissions rates for June were used for point sources in the Figures.

For NOx emissions, on-road mobile sources are dominant for Seoul, while point sources are dominant for Chungcheongnam-do. Except for Incheon and Ulsan, on-road and non-road mobile sources contribute large amounts of NOx emissions at large cities. Among 16 regions, Gyeonggi-do presents the highest NOx emissions rates of 552 tons/day, while Jeju-do shows the lowest NOx emissions rates of 41 tons/day in the CAPSS emissions inventory. NOx emissions from on-road mobile sources in Seoul takes 61 % of total NOx for the region, while NOx emissions from point sources in Ulsan explains 55 % of total NOx for the region.

For VOC emissions, area sources are the major contributors for all the regions except for Ulsan and Jeolanam-do, in which contributions of point sources are comparable to those for area sources. In Seoul, VOC emissions from on-road mobile sources amounts to 84 tons/day, taking 32 % of the total VOC emissions for the region, which is the highest VOC contribution from on-road mobile sources among all the regions.

For CO and PM10 emissions, on-road mobile sources show the largest contributions to the total emissions rates for each region. CO emissions from Seoul and Gyeonggi-do in the emissions inventory are 994 tons/day and represent ~ 40 % of nation-wide total CO emissions. Similarly, PM10 emissions from Seoul and Gyeonggi-do are 333 tons/day and explain 33 % of the nation total PM10 emissions. The nation-wide ratio of PM10 to NOx emissions for on-road mobile sources is 0.28, while those for Seoul and Gyeonggi-do are 0.59 and 1.02, respectively.

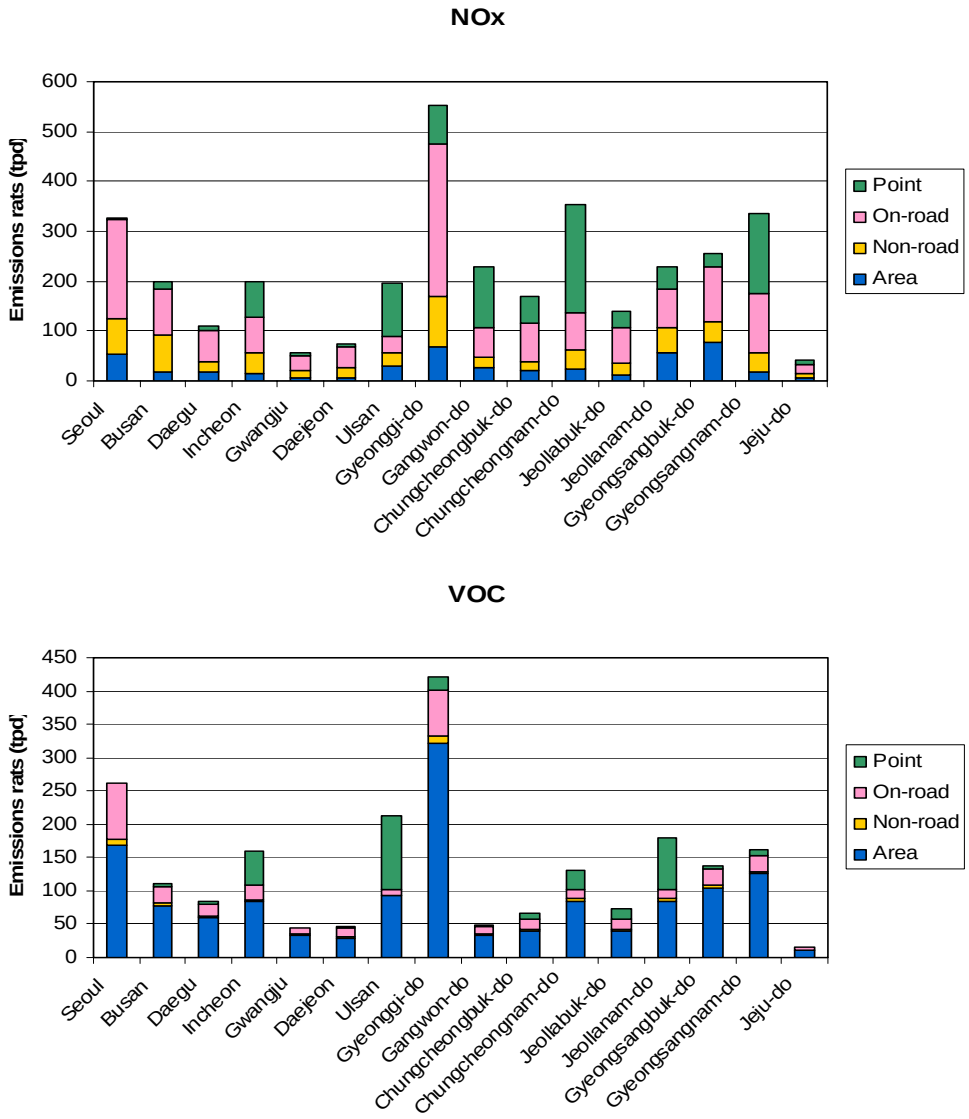


Figure 6.1 Regional emissions rates of NOx, VOC, CO, PM10, SOx, and NH_3 from each source type. Blue color represents area source emissions, yellow for non-road mobile, pink for on-road mobile, and green for point sources.

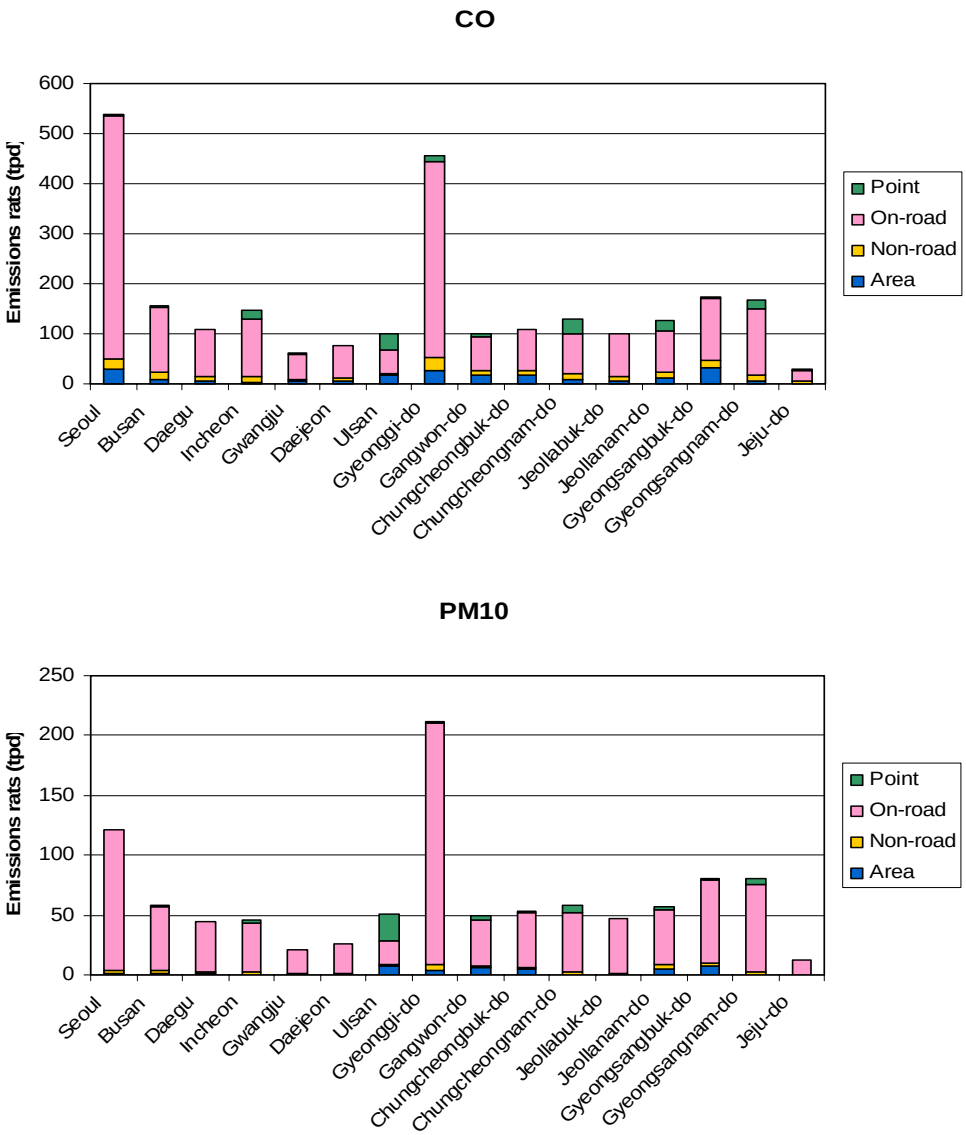


Figure 6.1 Continued

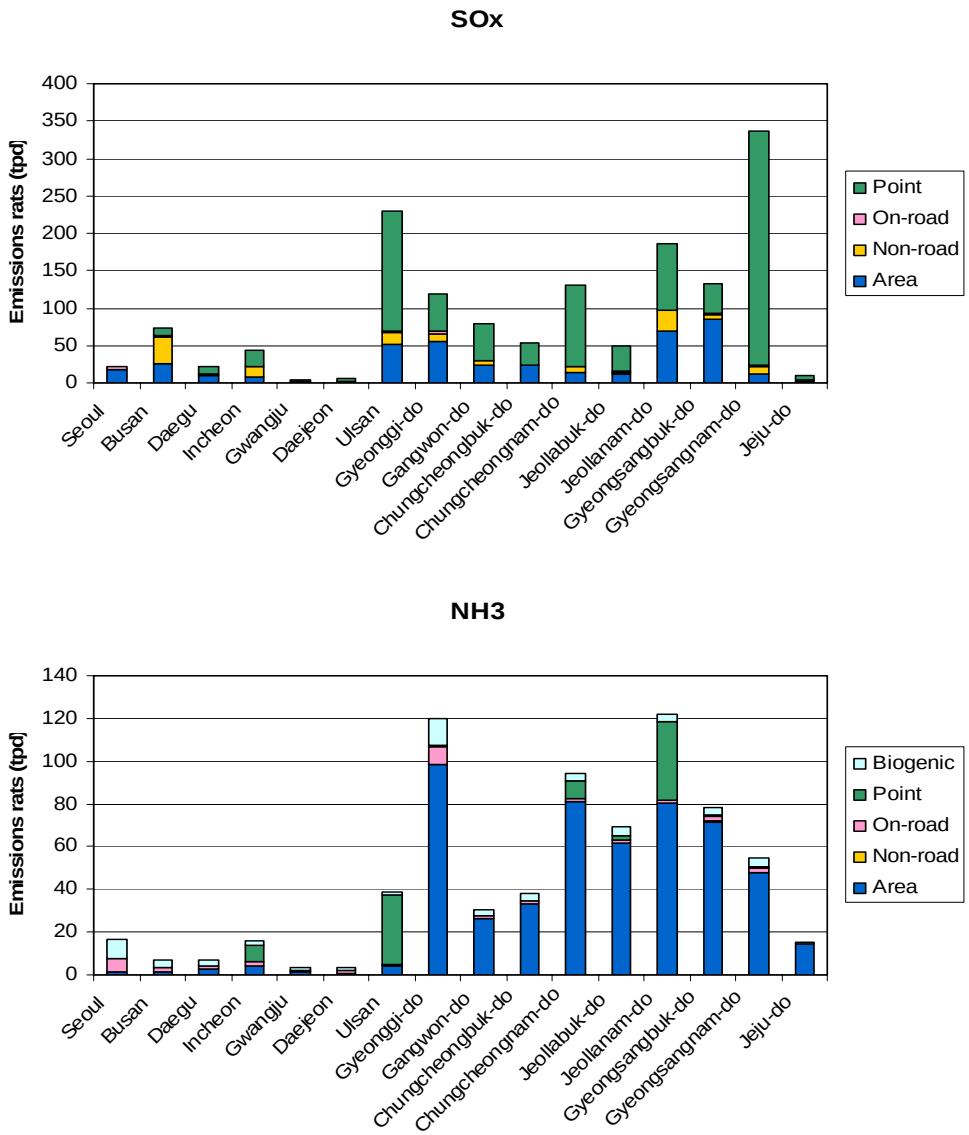


Figure 6.1 Continued

For SOx emissions, the point and area sources are the major contributors. While large cities show relatively low SOx emissions rates (~ 50 tons/day), Gyeongsangnam-do and Ulsan show 336 tons/day and 230 tons/day of SOx emissions, respectively, taking ~ 40 % of the nation-wide total SOx emissions.

NH3 emissions are very important for simulating particulate matter concentrations. Among four source types, area sources are the highest contributor to the emissions followed by point source emissions. Unlike other regions, on-road mobile and biogenic sources in Seoul and Gyeonggi-do become significant.

Ratios of VOC to NOx emissions in mass for each region and for individual source type are presented in Figure 6.2. When the VOC to NOx ratios are estimated with total emissions from all the sources, they are less than 1.0 for all the regions except Ulsan where high VOC emissions are available from point sources. When the ratio was calculated for area sources only, Gyeongsangnam-do shows the highest ratio of 6.8, while Gangwon-do and Gyeongsanbuk-do show the lowest ratios among 16 regions. It is noticed that the VOC/NOx emissions ratios for area sources are much higher than any other sources for all the regions with relatively high contributions to total VOC emissions sources. When compared to the ratio for Houston area (=3.0), large cities such as Seoul (=3.2) and Busan (=4.2) show comparable VOC/NOx emissions ratio for area sources.

For non-road mobile sources, the VOC/NOx emissions ratios for all the regions are ~ 0.1 which is lower than Houston area (~0.6) by a factor of 6. Similarly, the VOC/NOx emissions ratios for all the regions are ~ 0.2 for on-road mobile sources except in Seoul. The ratio in Seoul is ~ 0.4 and higher than other regions but still lower than the ratio for on-road mobile sources (~ 0.6) in the Houston area. It is supposed that the VOC/NOx emissions ratio for point sources vary with the source characteristics for a region. For example, the ratio for a petrochemical industry area would be higher than that for a region in which power plants are major point sources. Similarly CO/NOx emissions ratios are presented in Figure 6.3.

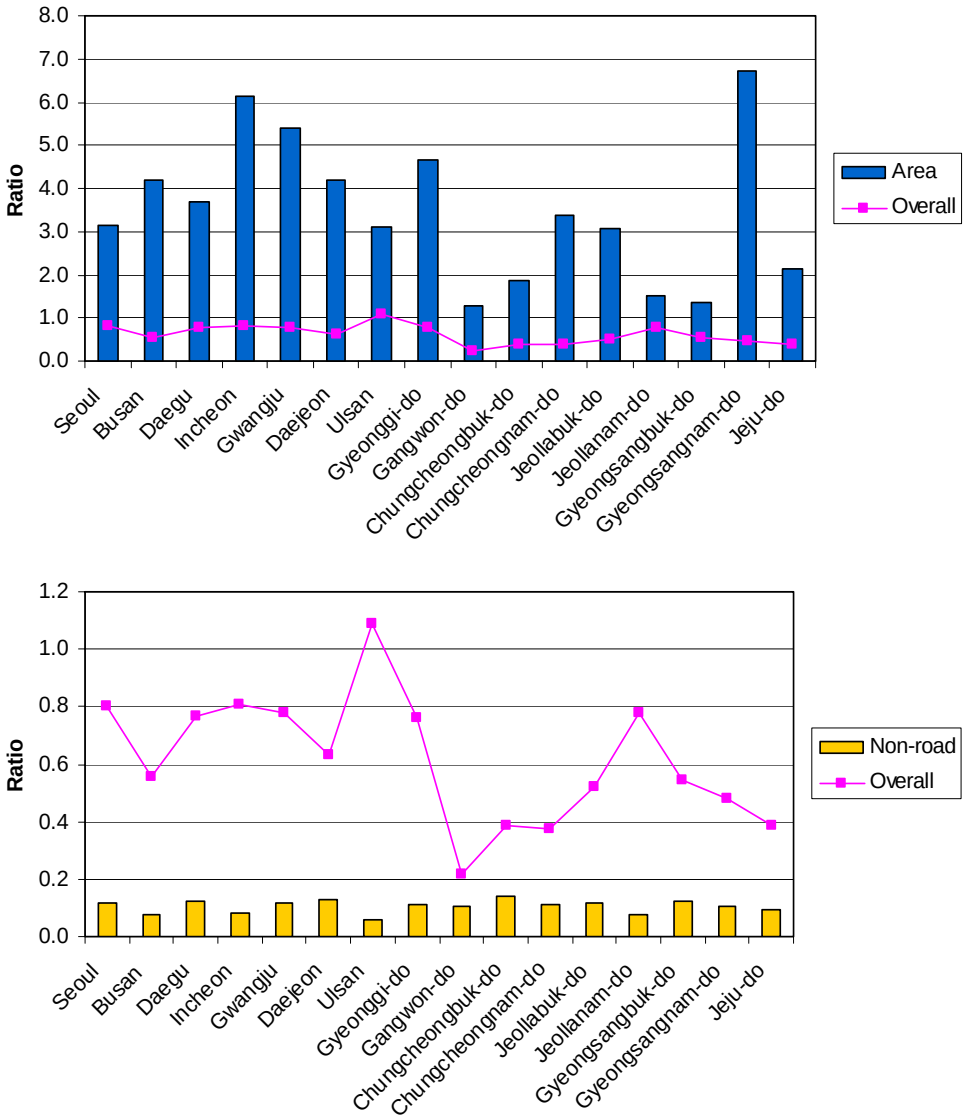


Figure 6.2 Ratios of VOC to NOx emissions for each region and for each source type; area, non-road mobile, on-road mobile, and point sources. Line plot represents the same ratio for emissions from all the sources.

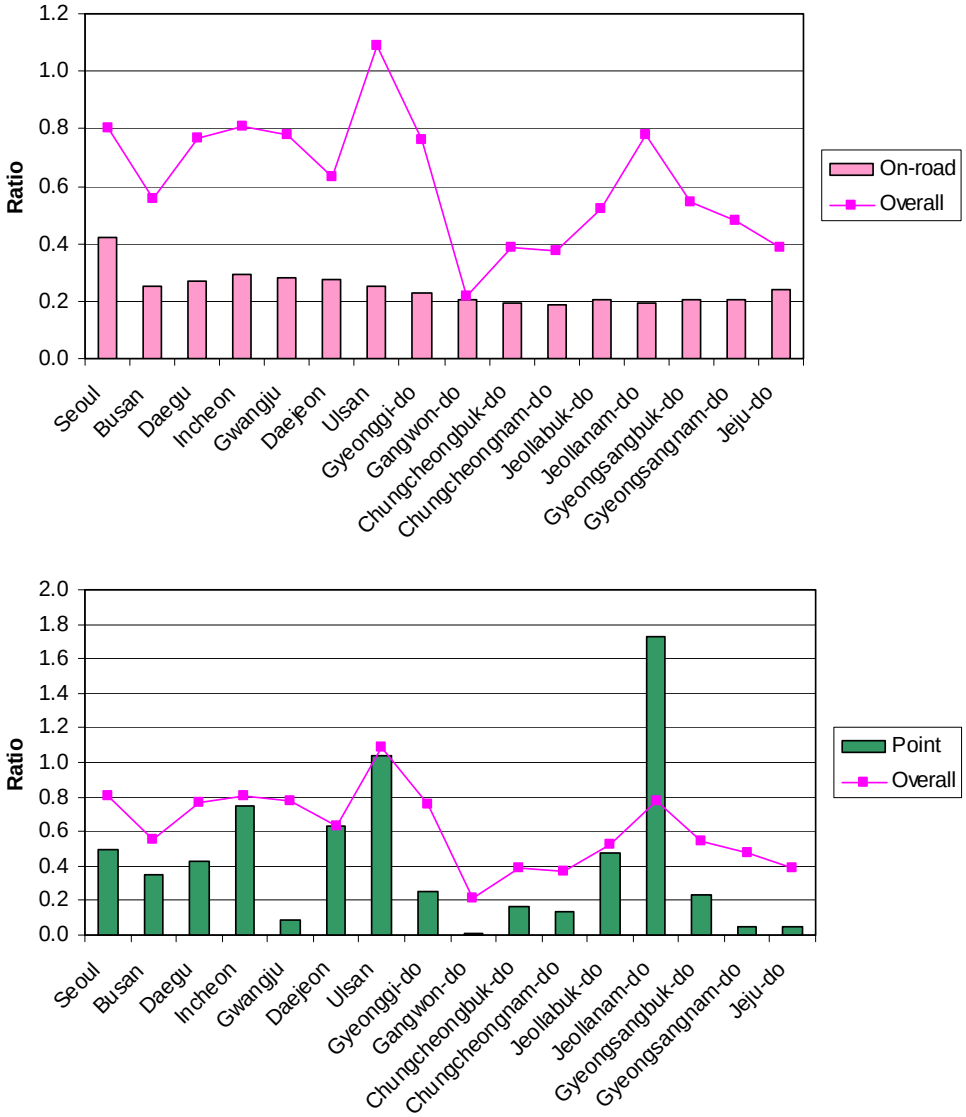


Figure 6.2 Continued

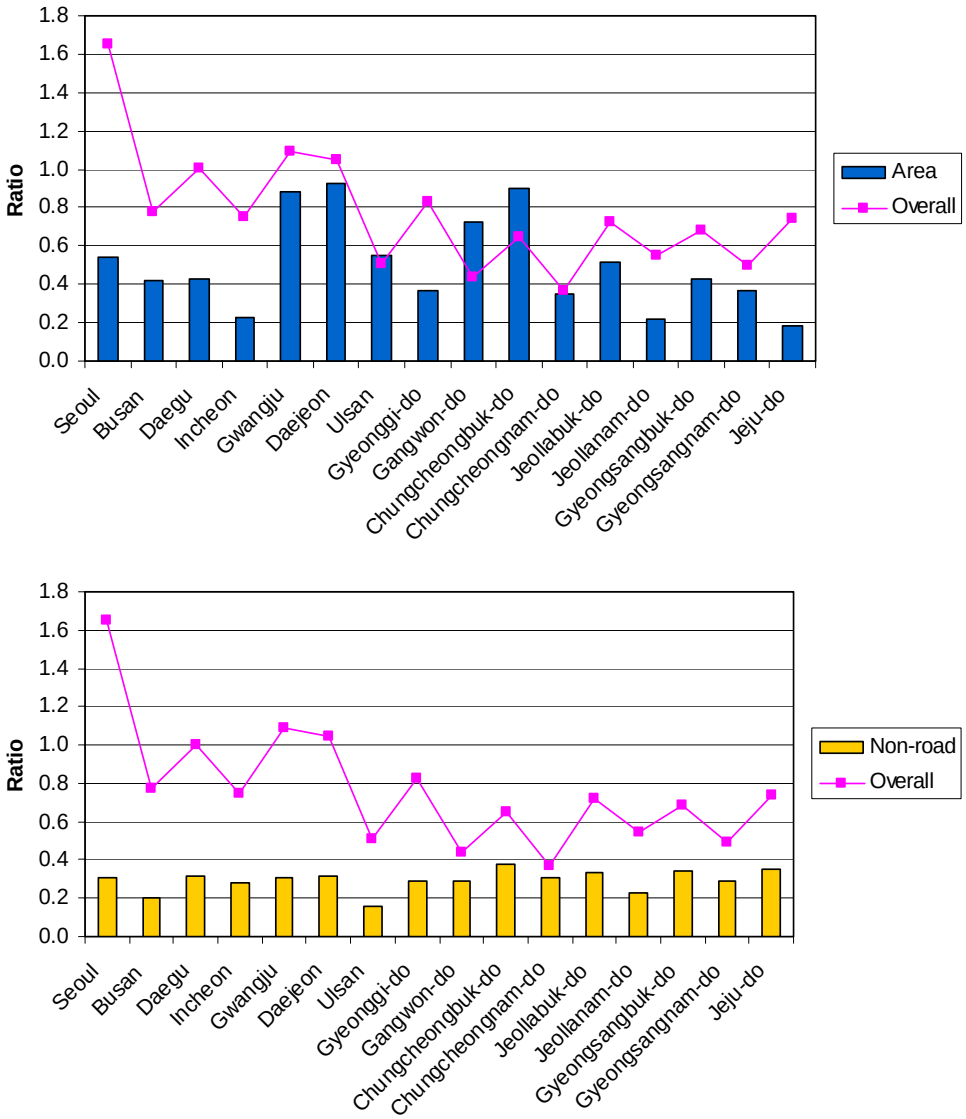


Figure 6.3 Ratios of CO to NOx emissions for each region and for each source type; area, non-road mobile, on-road mobile, and point sources. Line plot represents the same ratio for emissions from all the sources.

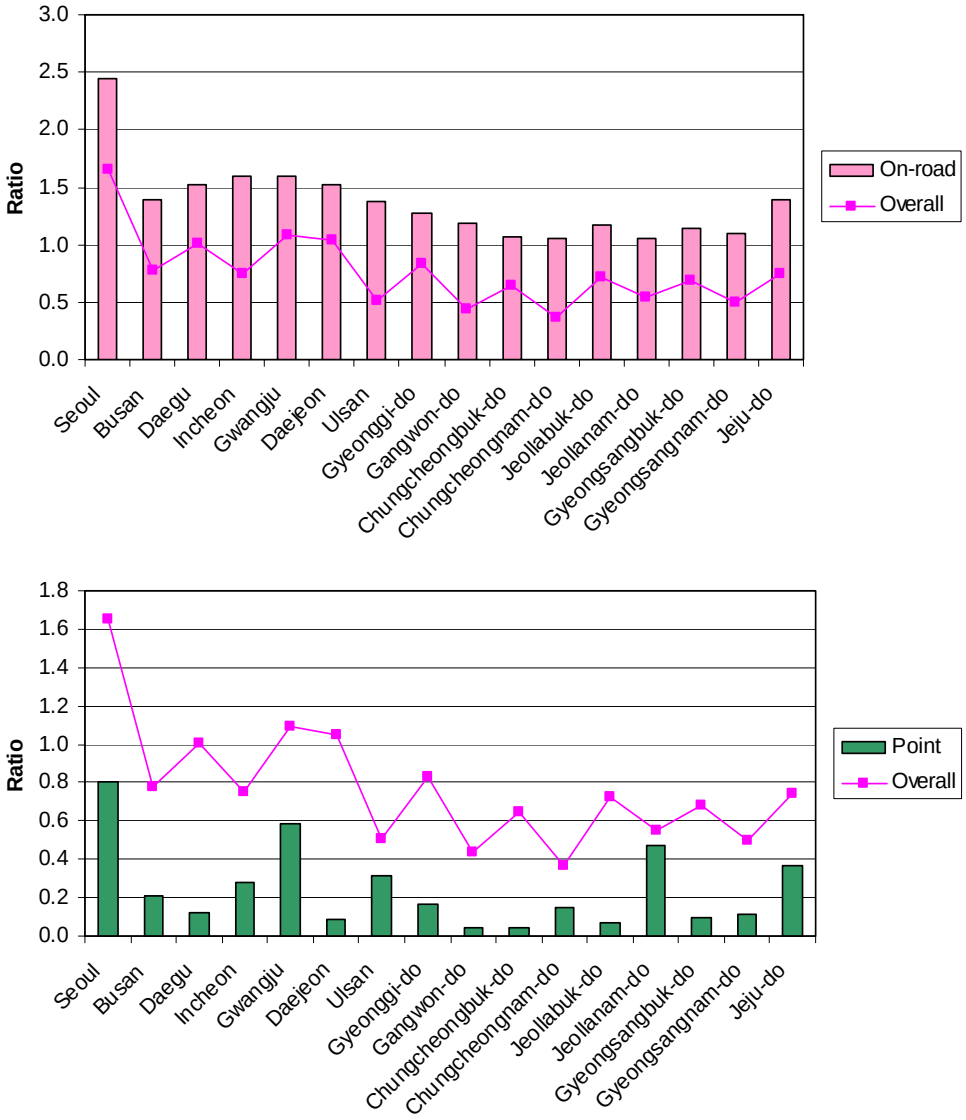


Figure 6.3 Continued

Figure 6.4 shows which source types emit large amounts of VOC emissions from area and point sources. Among area sources, VOC emissions from architecture coating are around 300 tons/day in the CAPSS emissions inventory, followed by coil coating and metal polishing processes. VOC emissions summed up for those three large area sources amount to 647 tons/day, taking about 50 % of total VOC emissions from all the area sources of which total VOC emissions are 1386 tons/day in the emissions inventory. It can be shown that the top 10 area sources contribute more than 80 % of total VOC emissions from all the area sources.

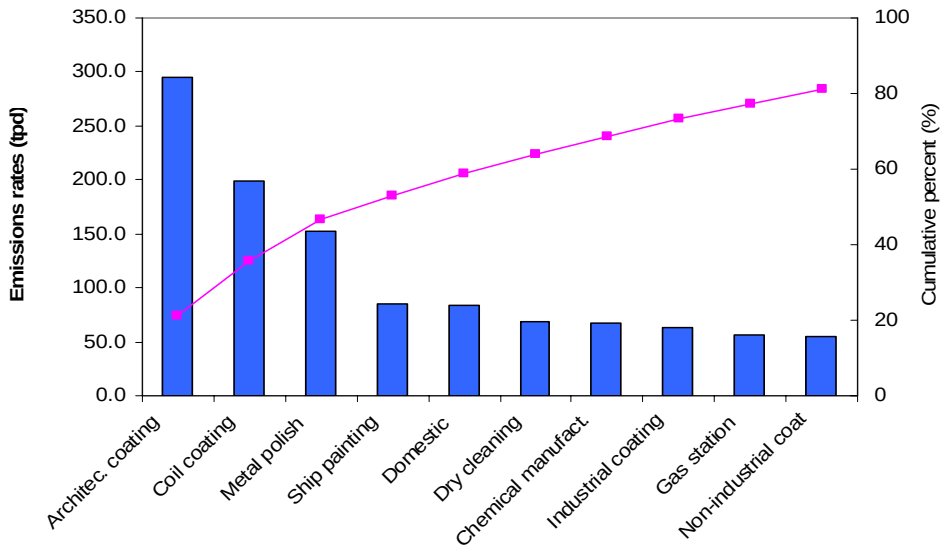
Among point sources, VOC emissions from petroleum products and storage were 147 tons/day, accounting 40 % of total point source VOC emissions, followed by industrial incineration and sugar manufacture of which VOC emissions are 75 tons/day and 42 tons/day, respectively. Those three large point sources and the top 10 point sources represent around 75% and 90 % of total VOC emissions, respectively, from all the point sources.

For on-road mobile sources, VOC emissions from passenger cars and taxies are 206 tons/day, representing ~ 55 % of total on-road mobile source VOC emissions, followed by heavy duty diesel vehicles including buses of which VOC emissions are 98 tons/day. It appeared that motorcycles show higher VOC emissions than light duty trucks and vans in the CAPSS emissions inventory. For VOC emissions from taxies and buses, it would be necessary to include chemical speciation factors for LPG and CNG combustion engines in the future work to represent chemical composition in a chemical mechanism selected better.

As shown in Table 3.4, around 500 SCCs are currently used in the CAPSS emissions inventory. As discussed previously, the SMOKE system largely depends on SCC to have the best match profiles for the chemical speciation, and temporal and spatial allocations. Also it is required to develop cross-reference tables and profiles for the processing steps to represent emissions characteristics better in Korea.

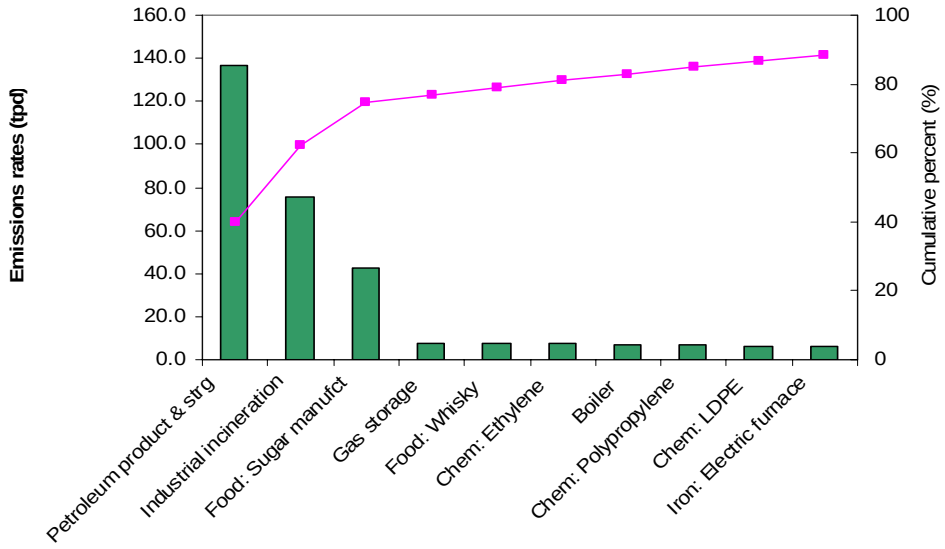
However it would be difficult to develop these internal databases for emissions processing for all the SCCs in a short time. After examining VOC emissions amounts for each source type in Figure 6.4 and 6.5, it is suggested to update internal databases for top 10 SCCs for area and point sources and

top 5 SCCs for on-road mobile sources first to minimize uncertainties during the emissions processing with minimum efforts. Characterization on emissions source should be carried out again for a selected modeling region because each region presents different emissions patterns associated with different industry, residential, and traffic environments.



(a)

Figure 6.4 Top-10 VOC emissions source classifications for area (a) and point (b) sources in CAPSS emissions inventory. Bars represent the emissions rate for each source classification, and lines for cumulative emissions in percentage.



(b)

Figure 6.4 Continued

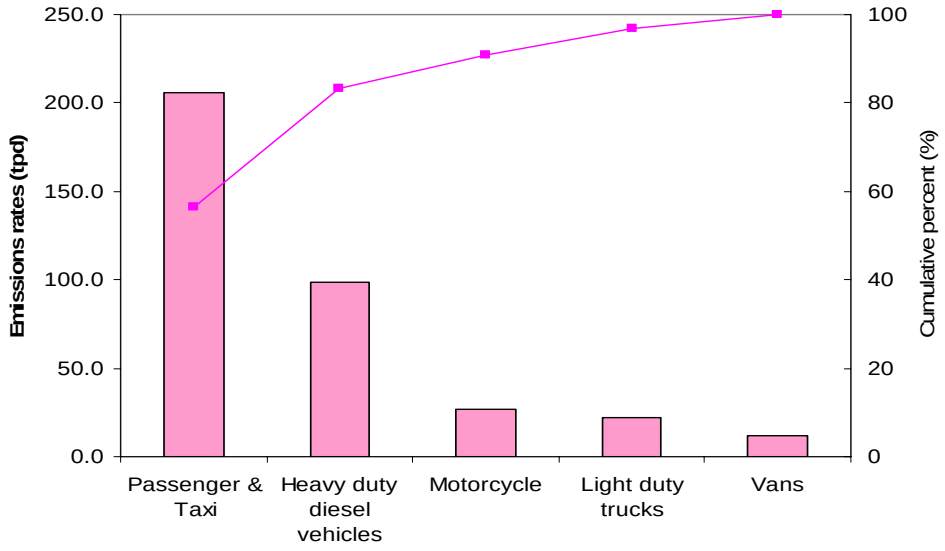


Figure 6.5 VOC emissions from on-road mobile sources in the CAPSS emissions inventory. Bars represent the emissions rate for each source classification, and lines for cumulative emissions in percentage.

Chapter 7. Discussion and Conclusion

Emissions are one of essential inputs to air quality modeling studies. It is required to prepare reasonable and reliable emissions inputs to better understand how air pollutants are emitted, transport, and react, and to correctly set up control strategies for a future state implementation plan. In order to provide air quality modelers with one way to use the CAPSS emissions inventory, the most updated emissions released by the MOE in Korea, for their air quality modeling works in the region, several tasks were planned and conducted in this year as follows;

- The CAPSS emissions inventory was converted to the IDA format for SMOKE processing. Separate input files for area, non-road/on-road mobile, and point sources were prepared with annual emissions rates from the emissions inventory.

- For point source emissions, monthly emissions files were also prepared to provide the users with an alternative to choose the emissions inputs. Stack parameters are available for each point source emissions to allow vertical distribution with a given meteorological condition.

- In the CAPSS emissions inventory currently available, around 500 SCCs are being used to characterize the sources. It is desirable to prepare internal databases for spatial allocation, chemical speciation, and temporal allocation during SMOKE processing to better represent the local emissions characteristics in the region for each SCC in the emissions inventory. At this moment, however, the information on the emissions inventory is not fully available. Thus, in this year, a SCC in the CAPSS emissions inventory was mapped to one of SCCs in the U.S. EPA to use the SMOKE-default cross-reference tables and profiles, assuming that source characteristics in Korea and the U.S. would be similar.

- To develop spatial surrogates for spatial allocation for a domain selected, a set of GIS shape files over Korea were collected from the U.S. EPA containing the emissions shape file for the region. Then, those GIS files were processed with the MIMS spatial allocator to prepare a spatial allocation factor for each county in the domain.

- After all the tasks above were done, the CAPSS emissions inventory was processed with SMOKE. To evaluate the CAPSS emissions inventory, SMOKE outputs were preliminary compared to each pollutant for each state based on the SMOKE report files.

Tasks for the next year are planned as follows;

- In principle, the internal databases in SMOKE will be updated for the CAPSS emissions inventory. The SCC mapping will be examined more thoroughly to check uncertainties that have been revealed from the procedure. Temporal variation profiles available for the CAPSS emissions inventory will be replaced with the default ones to better represent the diurnal variation. Surrogates for spatial allocation will be reviewed and updated with additional GIS shape files to have more reasonable horizontal distributions of the CAPSS emissions inventory.

- Before and after SMOKE processing, the CAPSS emissions inventory for Korea will be compared to ones for other countries (i.e., NEI from the U.S. EPA) for each source type and for each pollutant to check systematical uncertainties in the CAPSS emissions inventory.

- In addition to anthropogenic emissions, a processing procedure for biogenic emissions will be implemented. For the first time, land cover data for Korea, similar to BELD3 from the U.S. EPA, will be prepared to generate biogenic emissions through BEIS2 inside with meteorological data provided. After more comprehensive datasets

such as emissions factors and biomass density are gathered, we will try to move to BEIS3.

- It is assumed that there would exist an appreciable bias in predicted concentrations after air quality simulations with the CAPSS emissions inventory when compared to the observations. It would be difficult to address all weak points in the emissions inventory in this research, but we will try to come up with "rough" understandings on the emissions inventory after a few sets of CMAQ simulations.

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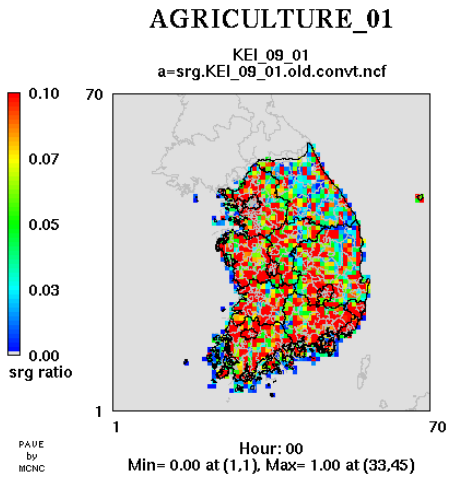
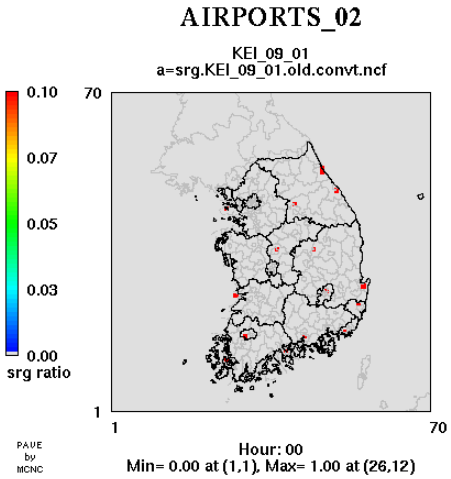
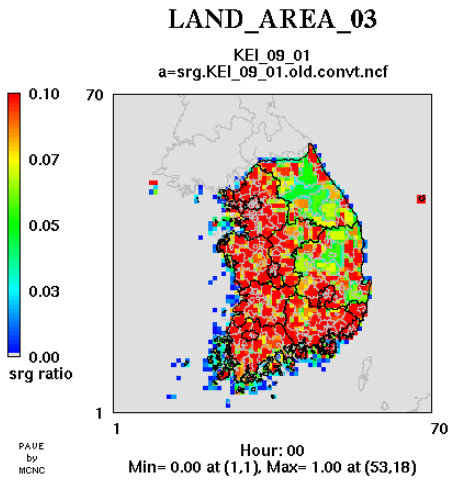
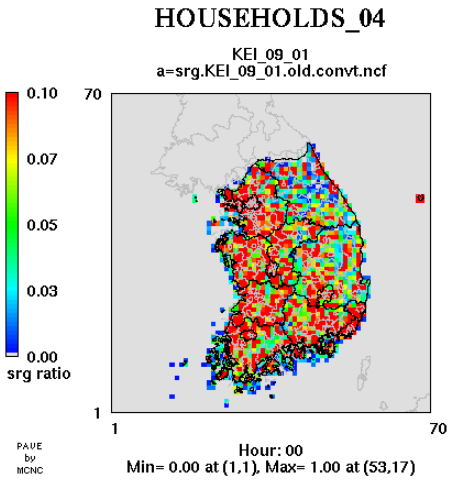
Appendix A. Surrogates for a 9-km resolved domain around Korean Peninsula.









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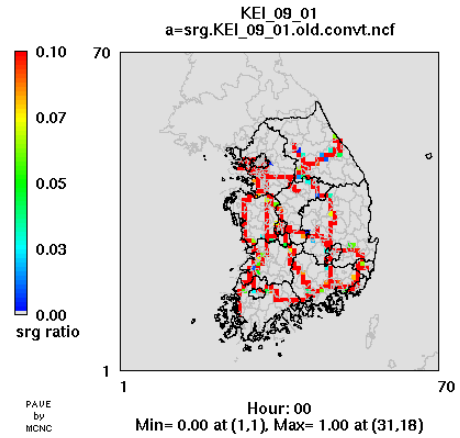

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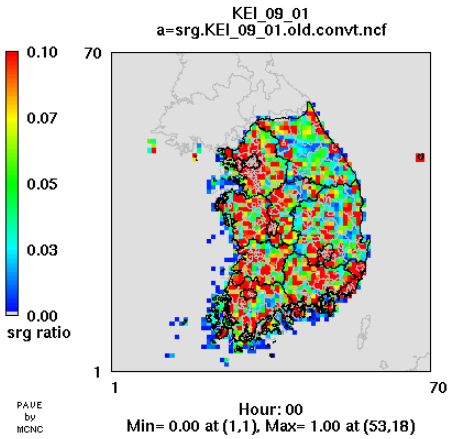

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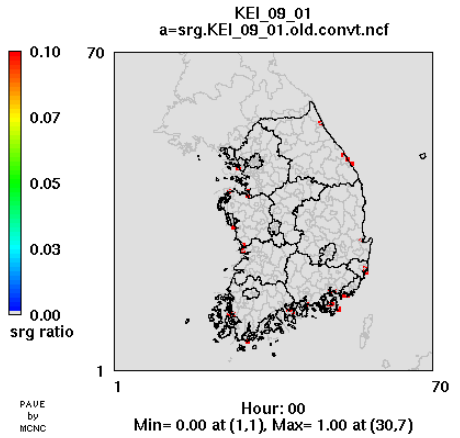

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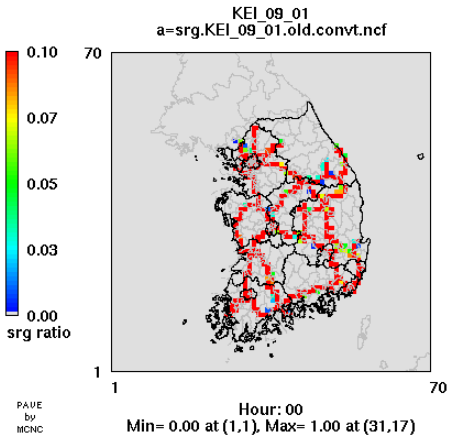

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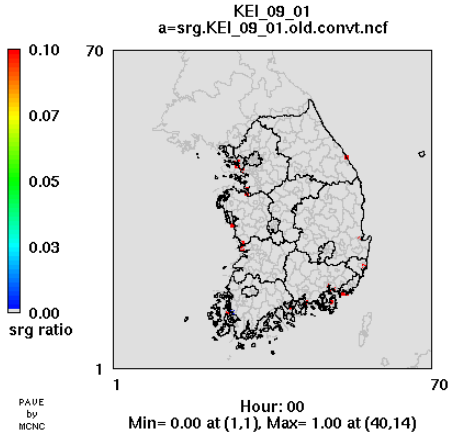

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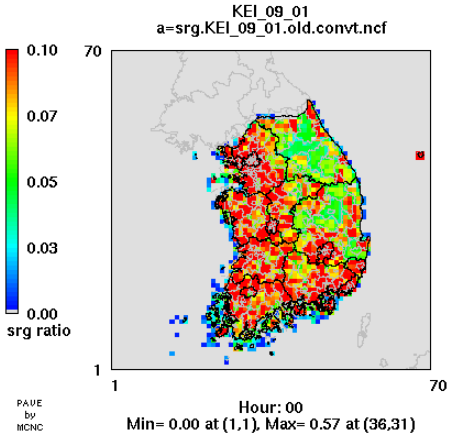

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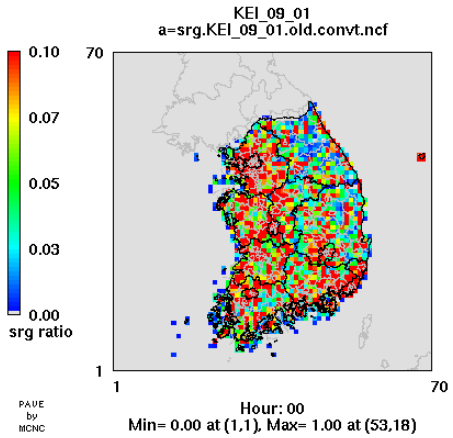
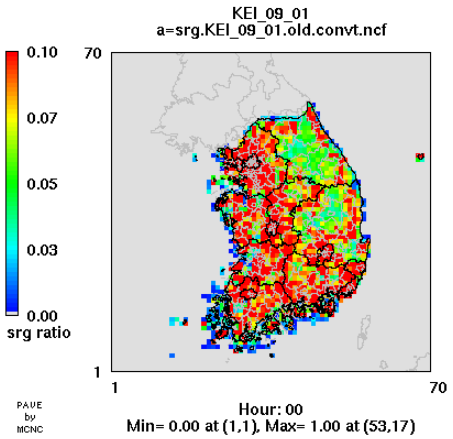
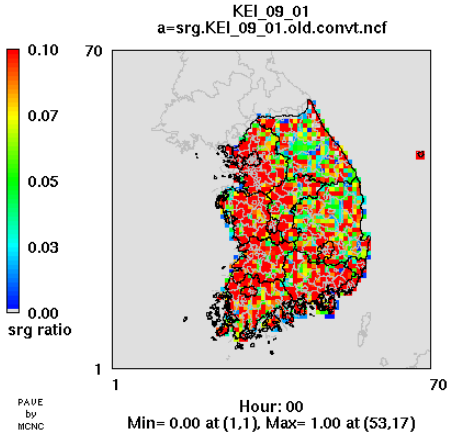


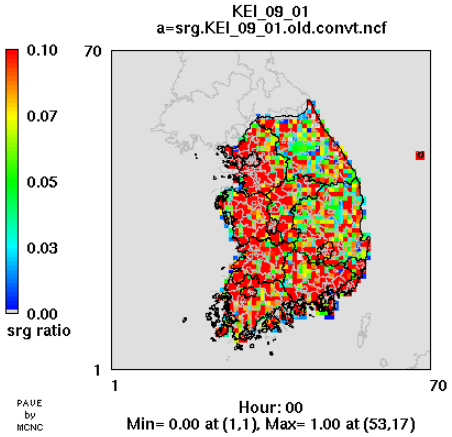
FOREST_14



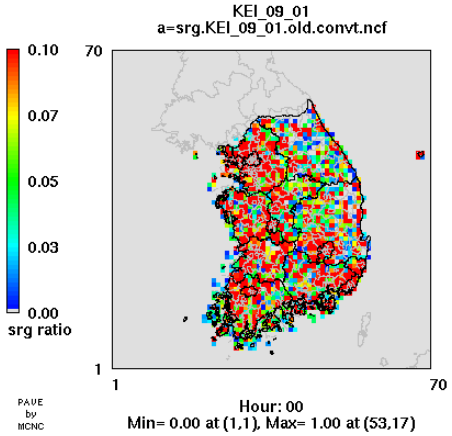
URBAN_PRI_15



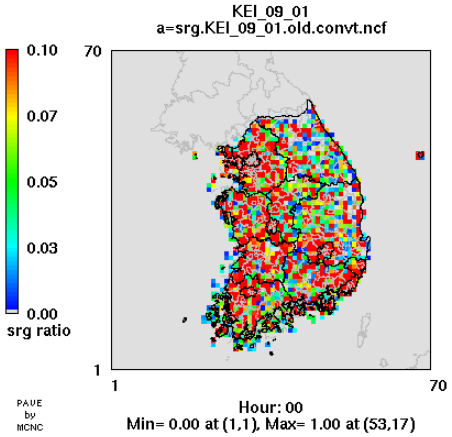
RURAL_PRI_16

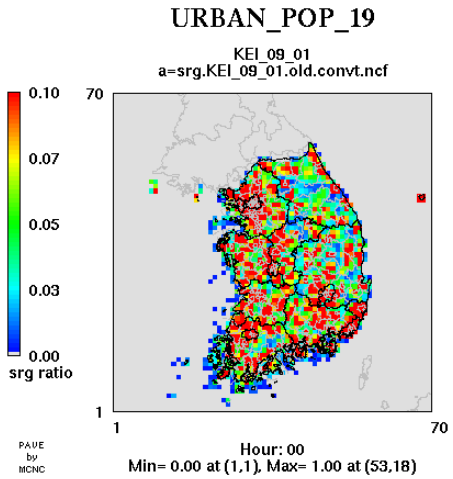


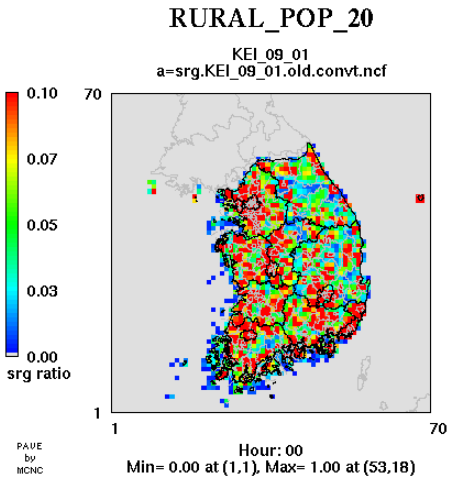
URBAN_SECND_17



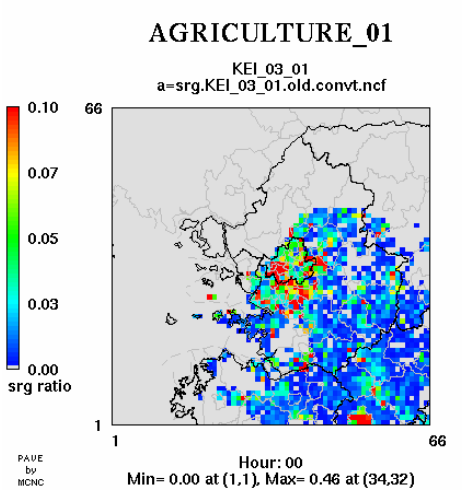
RURAL_SECND_18

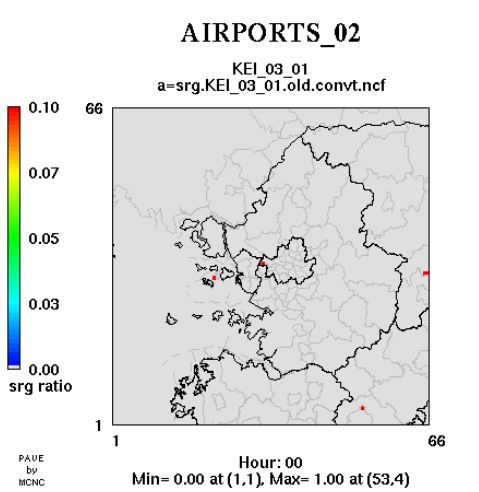


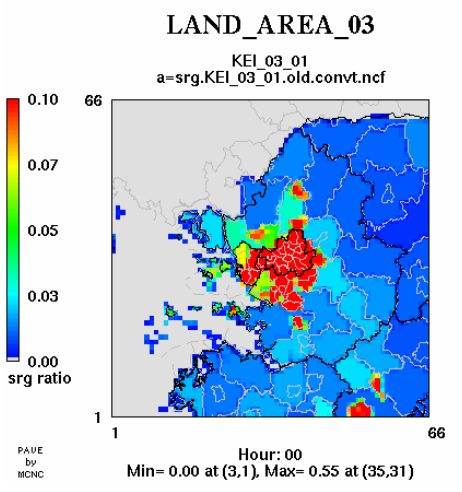

URBAN_POP_19
KEI_09_01
a=srg.KEI_09_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
70
1
1
70
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (53,18)

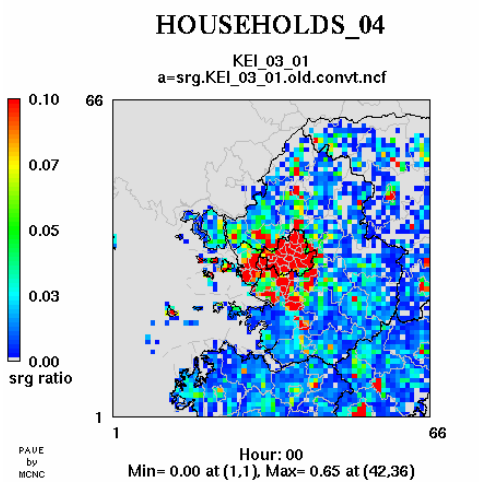

RURAL_POP_20
KEI_09_01
a=srg.KEI_09_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
70
1
1
70
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (53,18)

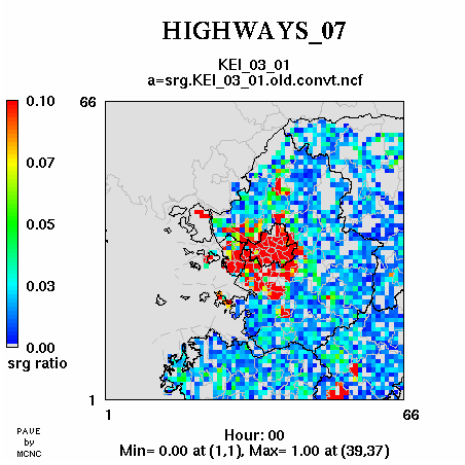
Appendix B. Surrogates for a 3-km resolved domain around Seoul metropolitan area

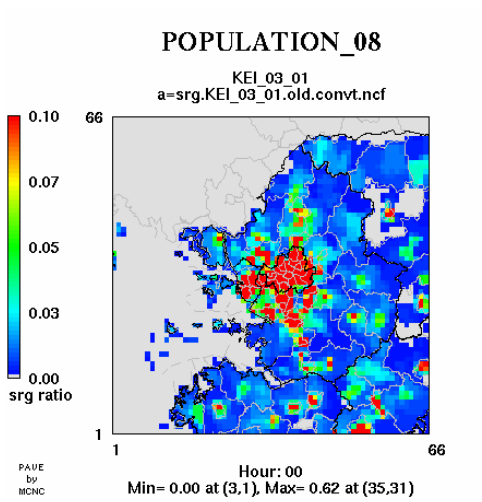


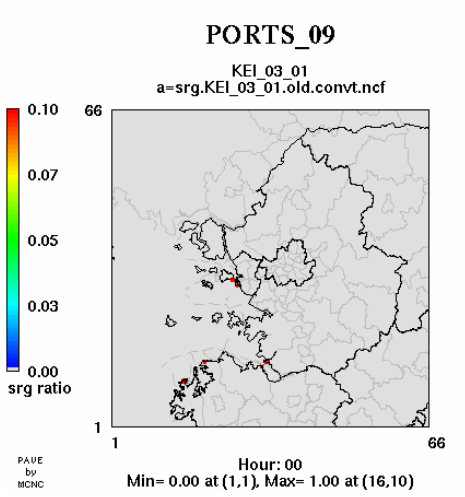


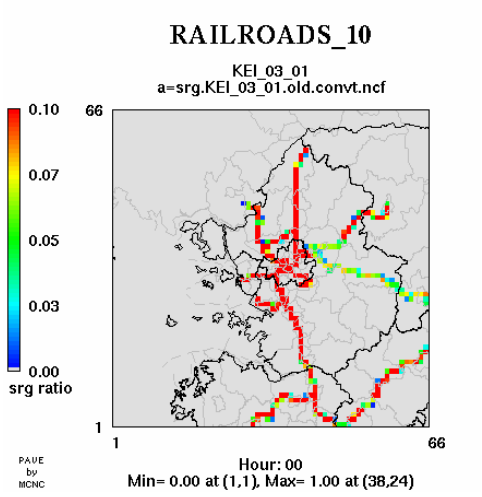


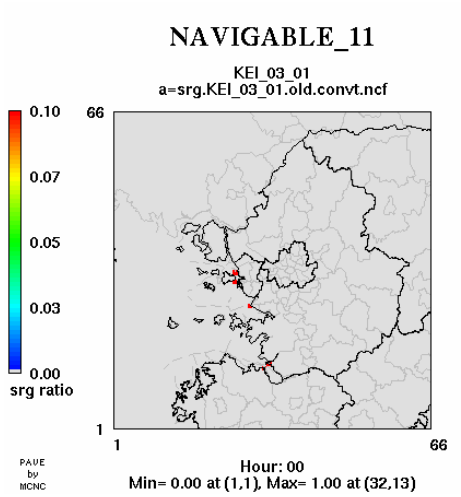


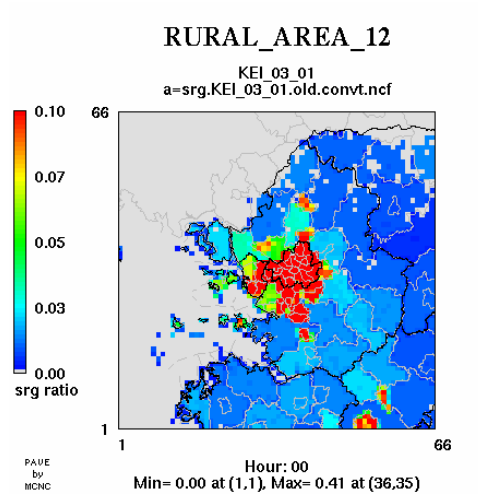

HIGHWAYS_07
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (39,37)

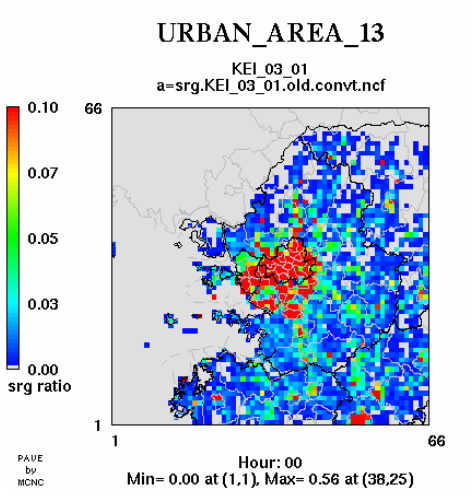

POPULATION_08
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (3,1), Max= 0.62 at (35,31)

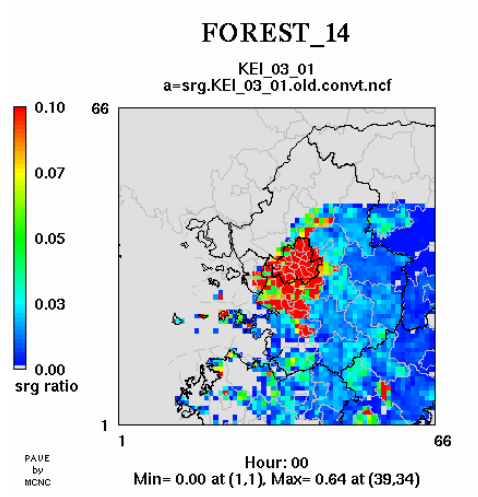

PORTS_09
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (16,10)

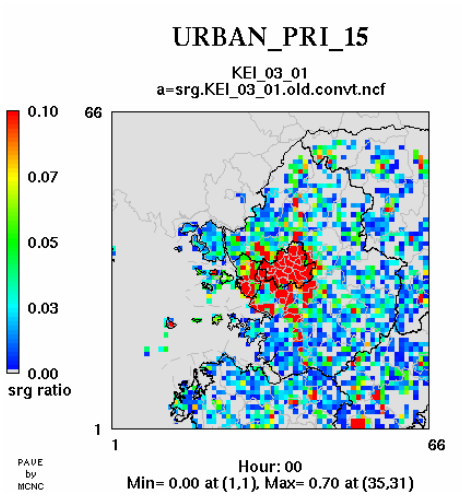

RAILROADS_10
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (38,24)

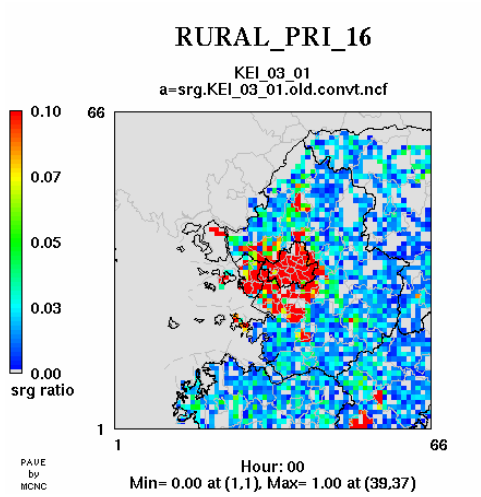

NAVIGABLE_11
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (32,13)

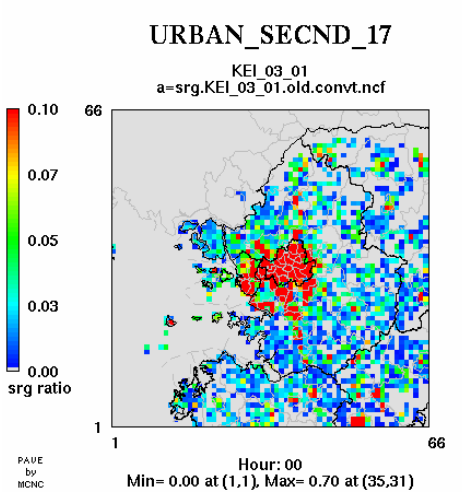

RURAL_AREA_12
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 0.41 at (36,35)

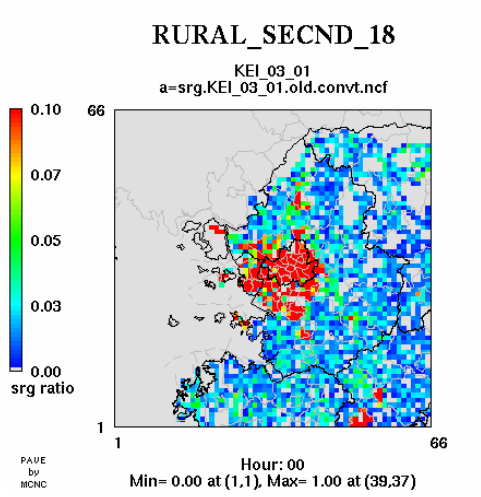

URBAN_AREA_13
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 0.56 at (38,25)

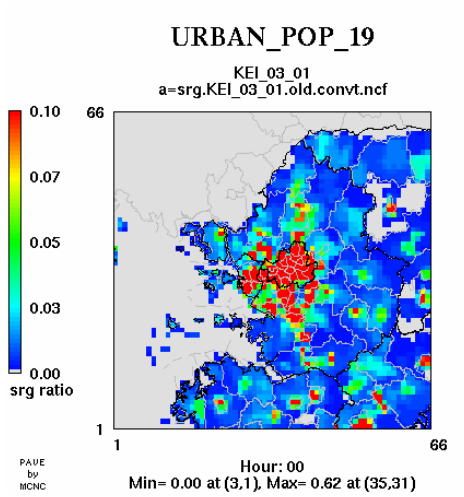

FOREST_14
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 0.64 at (39,34)

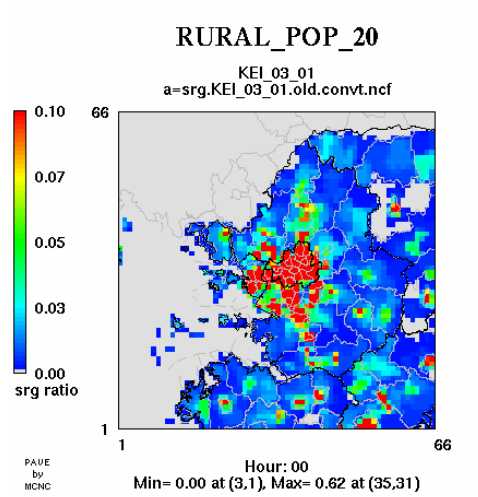

URBAN_PRI_15
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 0.70 at (35,31)


RURAL_PRI_16
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (39,37)


URBAN_SECND_17
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 0.70 at (35,31)


RURAL_SECND_18
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (1,1), Max= 1.00 at (39,37)


URBAN_POP_19
KEI_03_01
a=srg.KEI_03_01.old.convt.ncf
0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (3,1), Max= 0.62 at (35,31)


RURAL_POP_20
KEI_03_01
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0.10
0.07
0.05
0.03
0.00
srg ratio
66
1
1
66
PAVE
by
MCNC
Hour: 00
Min= 0.00 at (3,1), Max= 0.62 at (35,31)

국문요약 (Abstract in Korean)

상·하위 도시계획에 있어 보다 효율적인 대기질 관리를 위하여 각 개발 계획의 대안별 대기질 예측 및 평가가 요구된다. 현재까지 수행된 대기질 평가의 경우 배출총량을 고려한 환경용량 산정 연구가 실시 되지 않았으나, 향후 시행될 배출 총량제 도입 시에는 각종 계획 수립 시 대상영역의 배출량에 대한 환경용량 산정 및 평가는 필수적인 자료가 될 것으로 예상된다. 또한 사전환경성 검토 및 환경영향평가 시 오존, 미세먼지 등의 1차 및 2차 오염물질에 대한 영향예측을 실시하여야 하는 대상 지역 및 사업의 경우 반드시 대상영역의 3차원 기상장을 예측하고, 예측된 기상장을 이용한 배출량 산정 및 3차원 광화학 모델을 통한 대기오염 현상 규명을 위한 대기질 연구가 요구된다. 이에 따라 대기오염물질의 이류·확산, 수송, 반응 과정을 보다 잘 이해하고, 효율적인 대기 정책 수립을 위해서는 합리적이고 신뢰성 있는 배출 입력 자료의 확보가 대기질 모사 연구에 있어서 보다 중요한 요소로 대두될 전망이다.

현재 환경부에서 연구, 조사한 높은 신뢰도의 배출량 자료 (CAPSS, 2001, 2002, 2003)가 이용 가능함에도 불구하고, CAPSS 자료 자체를 대기질 모델링의 입력자료로 사용하기에는 여러 제한점이 제기된다. 이에 따라 CAPSS 자료를 국내 대기질 모델링에 활용될 수 있는 배출량 처리 시스템 개발이 시급한 실정이다. 미국의 경우, 국내 CAPSS 자료와 유사한 National Emission Inventory를 사용자가 이용할 수 있도록 하는 시스템을 개발하여 EPA 홈페이지에 공개하고 있으나, 국내에서는 이러한 범용적인 시스템이 구축되어 있지 않으므로 배출량 산정 시 사용자에 따라 서로 다른 결과가 나타나는 등의 어려움이 발생하고 있다. 이러한 문제점을 해결하기 위하여 본 연구에서는 CAPSS 자료로부터 시간 및 공간 할당 처리, 그리고 화학 메커니즘별 화학종을 구분하여 배출량을 산정할 수 있는 범용적 전처리 툴을 개발하고자 하였다.

본 연구에서 개발한 Korea Environment Institute-Emissions Inventory Preparation System(KEI-EIPS)는 CAPSS 자료를 대기질 모사 연구에 간편하고 보편적인 활용을 위한 것으로 배출원별 시간 할당, 공간 할당, 그리고 화학 메커니즘 별 화학종을 구분하여 배출량을 산정할

수 있는 전처리 툴이다. 공간할당의 경우 GIS 자료를 기반으로 하여 현재까지 도출된 최선의 기법을 사용할 수 있으며, 대기질 개선 정책 수립 시 적용 대상 지역과 이용 목적에 따른 배출량 변화를 예측한 대기질 모사가 가능하도록 설계하였다.

KEI-EIPS에서는 배출원별 특성을 고려하기 위하여 CAPSS 내의 약 500개의 배출원 분류코드(SCCs, Source Classification Codes)를 사용하였으며, 대상영역에 대한 공간할당을 위하여 국내 GIS 자료의 MIMS Spatial Allocator 을 통한 처리를 통해 각 지역에 해당되는 공간할당계수를 산출하였다.

개발된 KEI-EIPS의 활용성 평가를 위하여 1) PSU-NCAR/MM5를 사용하여 3차원 기상장 수치모의를 실시, 2) KEI-EIPS를 사용하여 CAPSS 자료의 시간, 공간 할당 및 화학종 분류 후 3차원 기상장 수치모의 결과와 SMOKE (Sparse Matrix Operator Kernel for Emissions) 를 적용하여 한반도 및 수도권 영역에 대한 배출량을 산정, 3) 3차원 대기질 모델인 CMAQ을 이용하여 수치모의 한 대기오염물질 농도와 대기오염측정망 자료의 비교를 실시하였다.

우선 SMOKE 결과 보고서를 사용하여 평가된 지역별 배출량 분포 등으로부터 KEI-EIPS 의 신뢰성을 검증하였다. CAPSS 자료를 이용해 모사된 대기오염물질 농도의 관측치와 비교, 그리고 배출원별 대기오염물질 배출 비율 등의 검토를 통해 현상황의 대기질 모사를 위한 배출량 자료의 불확실성이 확인되었으며, 이는 CAPSS 자료의 보완과 향후 연계될 과제를 통한 KEI-EIPS내의 내부자료 업데이트를 통해 개선되어 져야 할 것으로 사료된다.

본 연구에서 개발된 KEI-EIPS는 지금까지 존재하지 않아 발생했던 불편함을 해소하고 범용적으로 사용할 수 있는 공개 툴이라는 점과, 사용자들의 오류 보고 등을 통해 개선되고 엡그레이드 될 수 있는 기반을 갖춘 최초의 배출량 전처리 시스템이라는 점에 그 의의가 크다고 할 수 있다. 더욱이 지금까지 범용적인 툴이 존재하지 않아 동일한 자료를 이용한 대기질 연구임에도 불구하고, 사용자마다 다른 산정방법으로 인해 동일하지 않은 예측결과를 도출하게 되는 사례가 빈번히 발생하는 점을 고려할 때, 본 연구에서 개발된 툴은 산정된 국가 배출량 자료를 대기질 모사 연구에 이용할 수 있는 보편적이고, 상호확인 가능한 처리 방안을 제공함으로써 향후

대기질 예측 및 저감 대책 수립 시 예상되는 논란을 최소화 시킬 수 있을 것으로 기대된다.

끝으로 본 연구에 이어 연속되는 2차년도에서는 1차년도에서 개발된 KEI-EIPS의 내부 자료 업데이트 및 시스템 평가에 중점을 두어 보다 유용하고 신뢰성 있는 자료로 활용될 수 있는 시스템을 구축할 수 있을 것으로 기대된다.