

# **NATIONAL/REGIONAL AIR QUALITY MODELING ASSESSMENT IN CHINA USING AN ADVANCED AIR QUALITY MODELING SYSTEM**

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## **1. INTRODUCTION**

China is the world's most populous country with a fast growing economy that surges in energy consumption. It has become the second largest energy consumer after the United States although the per capita level is much lower than those found in developed or developing countries. More coal burned in power plants, more fuel used in industrial boilers and furnaces to meet the development of economy. The growing energy demand is consumed in up-soaring number of cars. The impact of the economy growth on the air quality is so severe that concentrations of most pollutants remain high in most industrial and metropolitan regions, such as Beijing, Shanghai, Tianjin, Shenyang and Fushun, despite the government efforts such as the enact of the Cleaner Production Promotion Law in June 2002 (Wang et al. 2001). Air pollution is damaging public health, air and water quality, agriculture and industry (Chameides et al, 1999; Hao et al., 2001; Physick, et al., 2001; Kato et al., 2002; Sorimachi et al., 2003). About 25% of China's total land area suffers acid rain in 1993 resulted from sulfur dioxide and soot caused by high sulfur-content fuel combustion (Terada et al, 2002).

Although there are some efforts on the simulation of acid deposition modeling in specific cities in China region, decision makers in China are hard to use those results to understand the formation of regional ozone, secondary particular matter (PM) and haze problems, to determine the adverse effects that causes human health and ecosystem, and even to design control strategies to improve their air quality. The U.S. Environmental Protection Agency has undertaken a study to conduct a regional modeling assessment by applying its premier modeling system, Models-3/CMAQ, to

the Great China region.

To conduct the first multi-pollutants modeling effort in China by Models-3/CMAQ, it is anticipated that obtaining the emission inventories over China will be a critical element for this study. According to the definition of the study domain, some parts of other countries around China need to be considered as well for their background contribution, such as Japan, South Korea, Korea DPR, Indonesia, Thailand, India and Mongolia. For this study we use the Asian emission inventory based on the emission estimates of the year 2000 to support the NASA TRACE-P program as our foundation. However, the emission database of TRACE-P was developed for a different purpose, further effort is required to transfer the emission inventories into the data format needed for the Models-3/CMAQ system. The further work of this study on the emissions preprocess includes the development of monthly, weekly and hourly variation profiles for the emissions in the study domain; the development of monthly emissions for January and July 2001; conversion of the major pollutant species into CB-4 format; and preparation of spatially gridded emissions according to the resolution and boundaries set up by the MM5 meteorological processing model. The China modeling domains are gridded at 36 km  $\times$  36 km and 12 km  $\times$  12 km grid resolutions, respectively.

The focus of this paper is the Models-3/CMAQ application to establish feasibility of model simulations over a large domain, i.e., covering the entire China and running the model for three seasons. This China modeling application is aimed at studying the formation and regional transport of ozone, PM and acid deposition, for selected episodes in 2001 in the non-transport and transport scenarios. The boundary conditions of background air concentrations and transported concentrations from outside of the China region are employed in the modeling runs separately. This application provides an understanding on the formation of regional ozone and haze problems for the policy makers in China, but provides the experience for agencies such as the State Environmental Protection Administration (SEPA) to refine the model and adapt it more thoroughly to conduct regional air quality management in China.

## **2. USEPA'S MODELS-3/CMAQ MODELING SYSTEM**

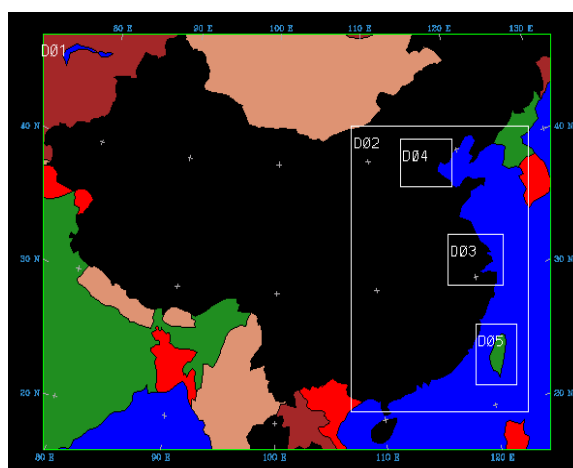
Over the past nine years, USEPA devoted major resources to developing an advanced modeling system with a "one-atmosphere" perspective, i.e., the U.S.EPA's Models-3/Community Multi-scale Air Quality (CMAQ) modeling system (Dennis, et. al., 1996; Byun, et. al., 1997; Byun and Ching, 1999; U.S.EPA, 1999). Models-3/

CMAQ is a numerical modeling system that can simultaneously simulate the transport, physical transformation, and chemical reactions of multiple pollutants across large geographic regions. The system is useful to states, other government and international agencies for making regulatory decisions on air quality management, as well as to research scientists for performing atmospheric research. It is a combination of Models-3, a flexible software framework, and the CMAQ modeling system for supporting air quality applications ranging from regulatory issues to scientific research on atmospheric processes. A modular science design of CMAQ allows the user to build different chemistry-transport models for various air quality problems. The “one-atmosphere” Models-3/CMAQ system was designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including ozone, particulate matter, visibility degradation, acid deposition, and air toxics, at multiple scales. The Models-3/CMAQ system was first released to the public in July 1998 and had a recent update release in September 2003 (U.S.EPA, 2003).

### 3. MODEL CONFIGURATION AND SETUP

#### Model Domain

In this Models-3/CMAQ application, the model domain covered the Great China region and in Figure 1. 36 km×36 km (D1) and 12 km×12 km (D2) grid resolutions set up by the MM5 meteorological processing model for episodes in 2001 used in USEPA’s Regional Air Quality Modeling in the Great China are used as the boundary conditions for this study.



**Figure 1.** Great China modeling domains

The domains had 130 x 94 horizontal grid cells using a 36-km resolution, 135 x 198 horizontal grid cells using a 12-km resolution resolution based on Lambert Conformal

map projection centered at (34<sup>0</sup>N, 102<sup>0</sup>E). Twelve vertical layers were configured initially following the Sigma ( $\sigma$ ) layer structure with denser grids at lower levels to better resolve the boundary layer. The  $\sigma$  -layer interfaces occurred at: 0.995 (38 m), 0.988 (92 m), 0.97 (230 m), 0.938 (482 m), 0.893 (846 m), 0.839 (1300 m), 0.777 (1850 m), 0.702 (2557 m), 0.582 (3806 m), 0.400 (6083 m), 0.20 (9511 m), and 0.00 (16,262 m).

### **Model Configuration**

The September 2003 release version of Models-3/CMAQ system was used in this modeling work. Further details of model configuration and science modules are given in Models-3/CMAQ science document and recent release note (U.S.EPA 1999 and 2003). The key science modules used in this modeling work are given below. Note that the selected science modules are the default options given in the September 2003 Models-3/CMAQ release version. The background initial and boundary conditions for the 36-km domain are based on available data to wash out the first three days during the model runs.

### **Model Inputs and Setup**

The Mesoscale Model Version 5 (MM5) v3.6 was used to provide meteorological input fields for the model simulations. The 36-km and 12-km domains and their meteorological outputs simulated by MM5 in the USEPA's Great Asia modeling effort were used in this work. The newest Meteorology/chemistry Interface Processor (MCIP) 2.2 that corrected layers collapsing released in June 2003 was used to process the raw MM5 output data into the format and structure required by the Models-3/CMAQ modeling.

### **Emission Estimates**

Inventories of 11 major chemical species have been developed by the TRACE-P project, including: SO<sub>2</sub>, NO<sub>x</sub>, CO<sub>2</sub>, CO, CH<sub>4</sub>, non-methane volatile organic compounds (NMVOC), black carbon aerosol (BC), organic carbon aerosol (OC), NH<sub>3</sub>, PM<sub>10</sub> and PM<sub>2.5</sub>. Detailed emissions are considered by type of fossil fuel for the sectors of anthropogenic combustion, which are aggregated into five primary source categories of industry, residential, transportation, power generation, and agricultural. Biomass burning is calculated independently in three major categories: forest burning, savanna/grassland burning and the burning of crop residues. Emission inventories are updated to year 2000 for each country in Asia and for each province of China and the other countries.

Annual total emissions of 11 pollutants with 18 subcategories of NMVOC are developed by the TRACE-P project. This is not directly compatible with the needs of Models3-CMAQ, which requires the CB-4 chemical mechanism as 22 species. Different species of NMVOC will be merged into ALD2, ETH, FORM, OLE, PAR, TOL and XYL; PM2.5 and PM10 will be divided into fine aerosols in light of the speciation profile developed by USEPA (used by the SMOKE model as files GSPRO and GSREF) as shown in Table 1; and biogenic ISOP and TERPB will be directly prepared by GIS based on land-use information. Only domestic, agricultural, biomass burning, and biogenic sectors are assumed to have seasonal variation in China in the TRACE-P project. Monthly operation hours of stoves for domestic heating will be estimated based on monthly mean temperatures for each province in China. Combustion emissions for the domestic sector in January and July will be estimated based on the monthly profiles of stove hours. The weekly and hourly profiles developed by USEPA will be further adjusted based on the understanding of economic activities and living habits in China.

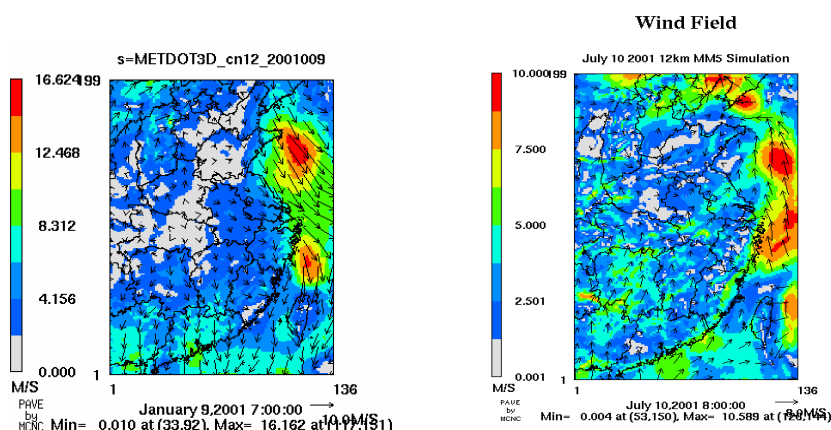
**Table 1:** TRACE-P classes mapped to CB-IV

No	Trace-P Pollutant	MW	Mapping from Trace-P to CB4	CBIV(22)
1	Ethane	30.0	$2*[9] + 2.5*[16] + 1.5*[31]$	ALD2
2	Propane	44.0	[23]	CO
3	Butanes	58.0	[6]	ETH
4	Pentanes	72.0	[15]	FORM
5	Other Alkanes	86.0	[30]	ISOP
6	Ethene	28.0	[27]	NH3
7	Propene	40.0	$0.9*[21]$	NO
8	Terminal Alkenes	56.2	$0.1*[21]$	NO2
9	Internal Alkenes	56.2	$1.6*[1]+1.5*[2]+1.5*[10]+[24]+0.5*[32]$	NR
10	Acetylene	26.0	$[7]+[8] + 0.5*[32] + 0.5*[31]$	OLE
11	Benzene	78.0	$0.4*[1]+1.5*[2]+4*[3]+5*[4]+6*[5]+[7]+2*[8]+1.5*[10]+8.5*[32]+[11]+4*[17]+1.33*[19]+6*[31]$	PAR
12	Toluene	92.0	[25]	PEC
13	Xylenes	106.0	[29]-[28]	PMC
14	Other Aromatics	117.0	[28]-[25]-[26]-PNO3-PSO4	PMFINE
15	HCHO	30.0	[28]*x	PNO3
16	Other Aldehydes	88.0	[26]	POA
17	Ketones	126.0	[28]*x	PSO4
18	Halocarbons	150.0	[20]	SO2
19	Other	72.0	$0.02*[20]$	SULF
20	SO2	64.0	[31]	TERPB
21	NOx	46.0	$[12] + 0.5*[14]$	TOL
22	CO2	44.0	$[13] + 0.5*[14]$	XYL
23	CO	28.0		
24	CH4	16.0		
25	BC	12.0		
26	OC	12.0		
27	NH3	17.0		
28	PM2.5		Note: x will depend on sectors of SCC	
29	PM10			
30	ISOP (biogenic,GEIA)	5 carbons		
31	TERP (biogenic,GEIA)	10 carbons		
32	Other VOC (biogenic,GEIA)	10 carbons		

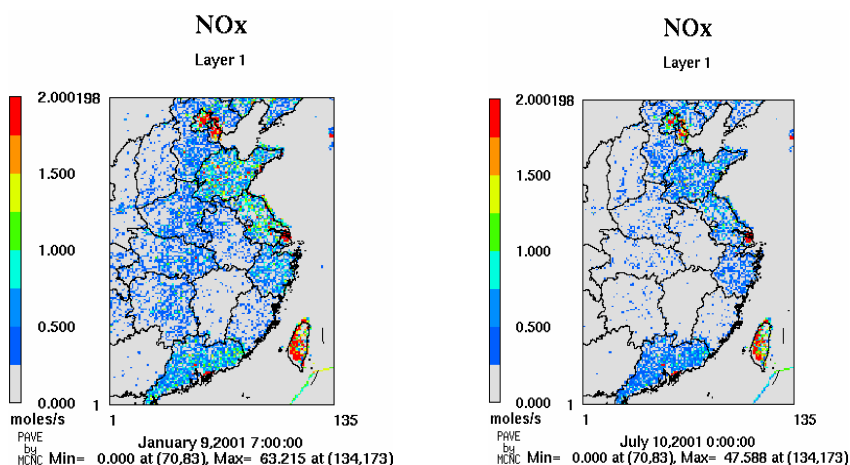
## 4. RESULTS AND DISCUSSIONS

The objective of this study was to conduct model results on January and July 2001 scenarios. Examples of wind fields of MM5 outputs are shown in Figure 2 in January and July 2001. The boundary conditions (BC) are set to a set of background

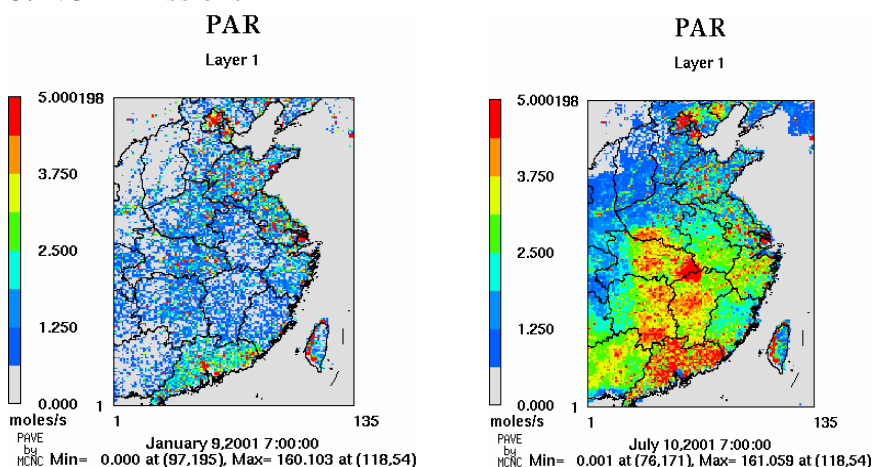
concentrations such as 35 ppb in the first layer for ozone. Results from the Models-3/CMAQ simulation are discussed below. The discussion first focused on the effects of transported pollutants such as Ozone, fine PM 2.5 and visibility and major PM 2.5 constituents such as sulfate PM and nitrate PM. As part of a series of on-going modeling efforts, January and July 2001 episodes Models-3/CMAQ simulation over



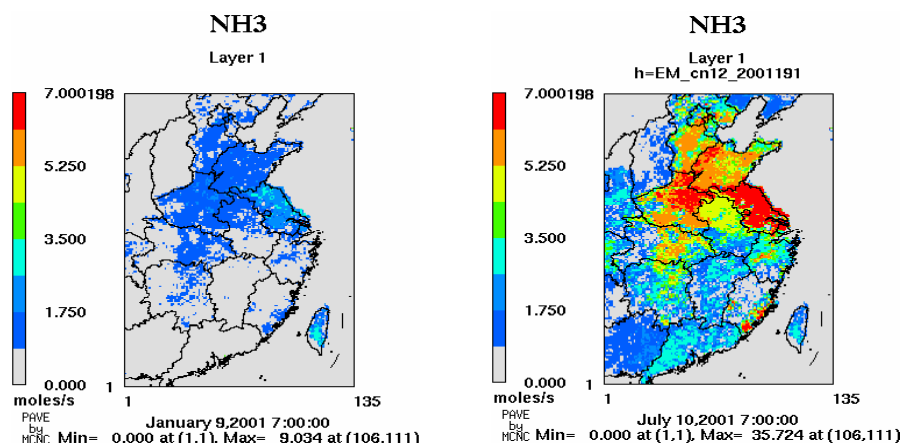
**Figure 2. Wind Fields**



**Figure 3. NOx Emissions**



**Figure 4. Paraffin Emissions**



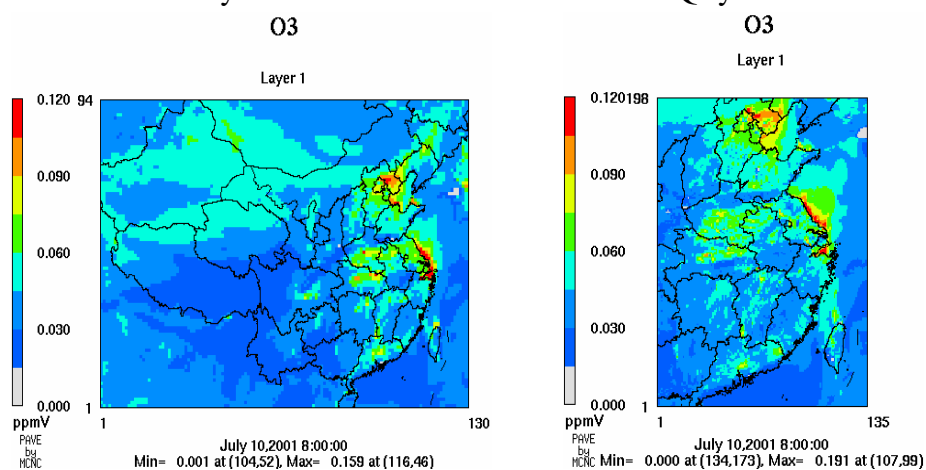
**Figure 5.** NH<sub>3</sub> Emissions

China was conducted. The examples of NO<sub>x</sub>, Paraffin and NH<sub>3</sub> emissions are shown in Figures 3-5. Results showed that the Models-3/CMAQ system was capable of simulating key criteria pollutants reasonably well over a typical day and within an acceptable run time for ozone and PM<sub>2.5</sub>. Concentrations Ozone, PM<sub>2.5</sub> and visibility from CMAQ simulations were shown in Figures 6-8 for 36km and 12km domains. Ozone and PM<sub>2.5</sub> concentrations are higher in suburban of Beijing and Shanghai associated wind directions. We use the trend of emissions in “what if” case study. There are three “what if” cases, the base case, 50% increased emissions case and 50% decreased case. The results of “what if” cases shown how emissions will improve or worsen the air quality in China as Figures 9-11. The ozone concentrations are different the background of ozone concentration from the nesting boundary which is transported from outside (36km domain) of the region based on the wind field of the MM5 output. The ozone concentrations are 80-120 ppb in Beijing and 100-160 ppb in Shanghai. The PM<sub>2.5</sub> episode average is 40 ug/m<sup>3</sup> in Beijing area and 22 ug/m<sup>3</sup> in Shanghai.

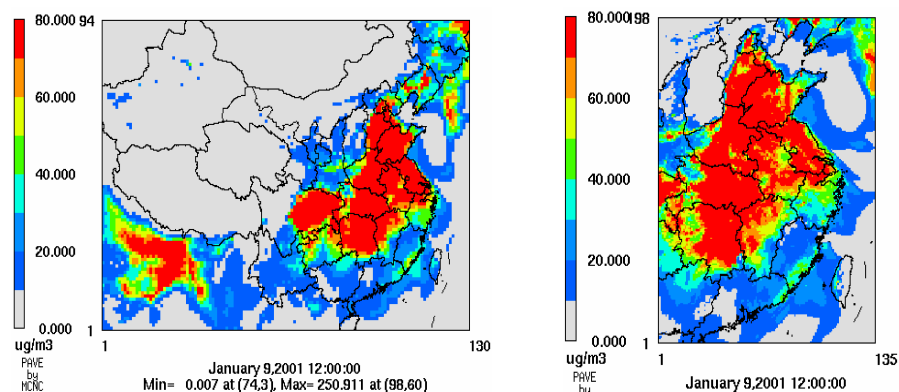
## 5. SUMMARY

Using an advanced air quality modeling system such as USEPA’s Models3/CMAQ, the “One Atmosphere” model, we are able to assess multi-pollutants at once such as ozone, particulate matter, acid deposition, and visibility. The Models3/CMAQ is conducted with the air quality assessment applications in Asia countries (Fu, et al., 2003). A pilot study using Models-3/CMAQ has been conducted over Asia (36-km), Regional (12-km) to simulate multi-pollutants, including primary and secondary pollutants such as ozone, PM, acid deposition, visibility, SO<sub>2</sub>, NO<sub>x</sub>, etc. The results (January and July case) seemed to show lower O<sub>3</sub> than expected. High PM<sub>2.5</sub> were simulated over metropolitan areas with

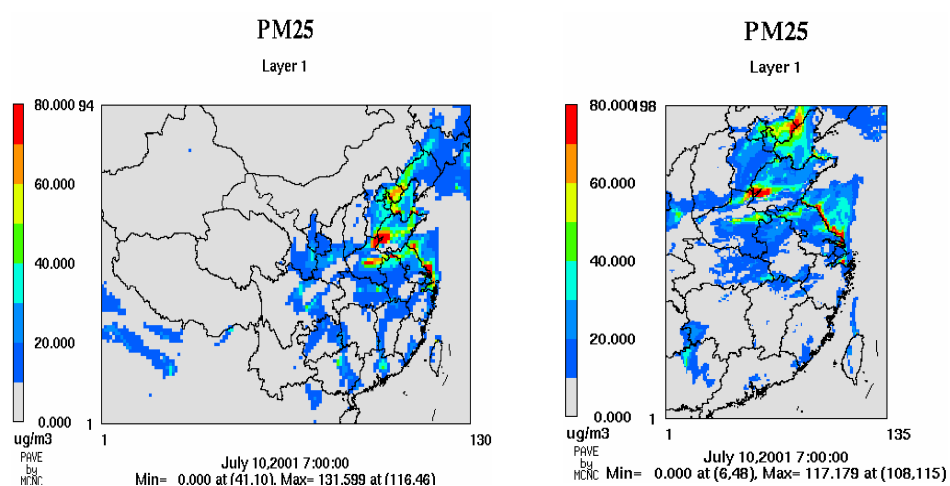
significant secondary constituents. The Models-3/CMAQ system can be a useful



**Figure 6.** O<sub>3</sub> concentrations: 36km and 12 km domains (July 2001)

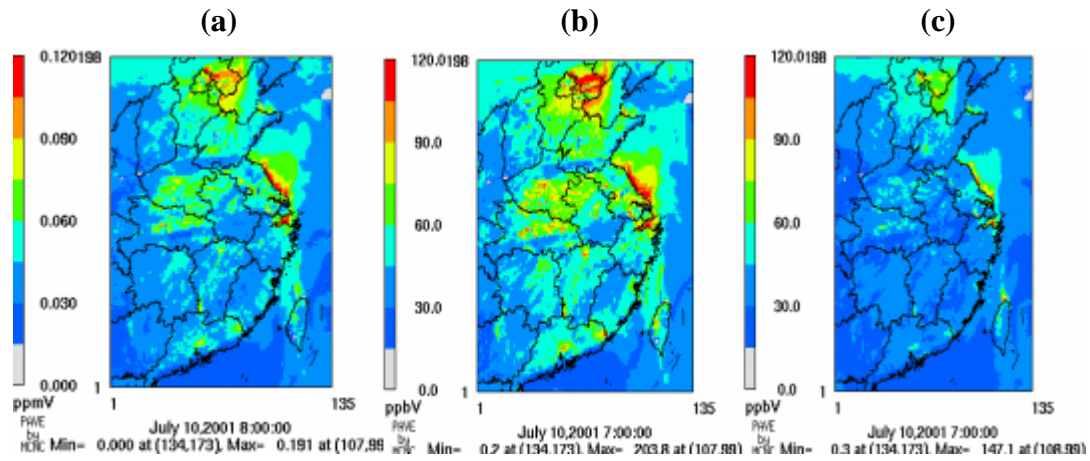


**Figure 7.** PM2.5 concentrations: 36km and 12 km domains (January 2001)

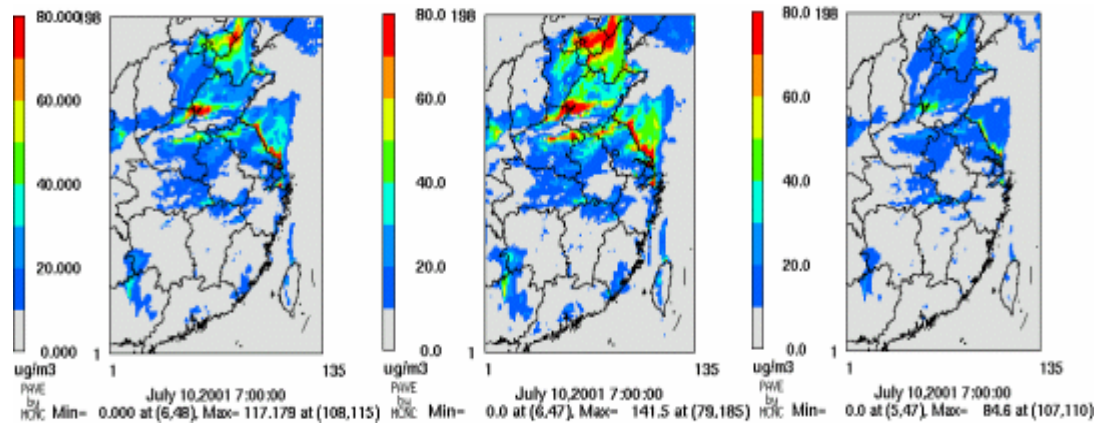


**Figure 8.** PM2.5 concentrations: 36km and 12 km domains (July 2001)

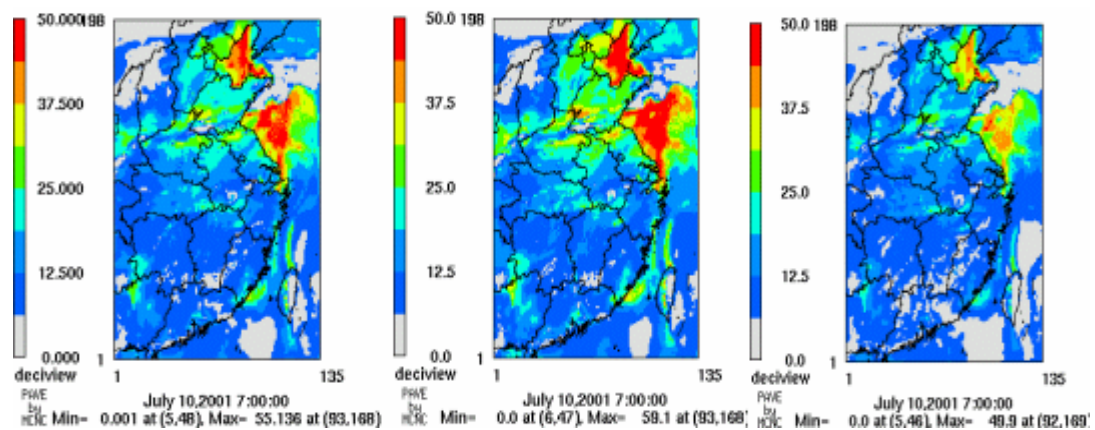




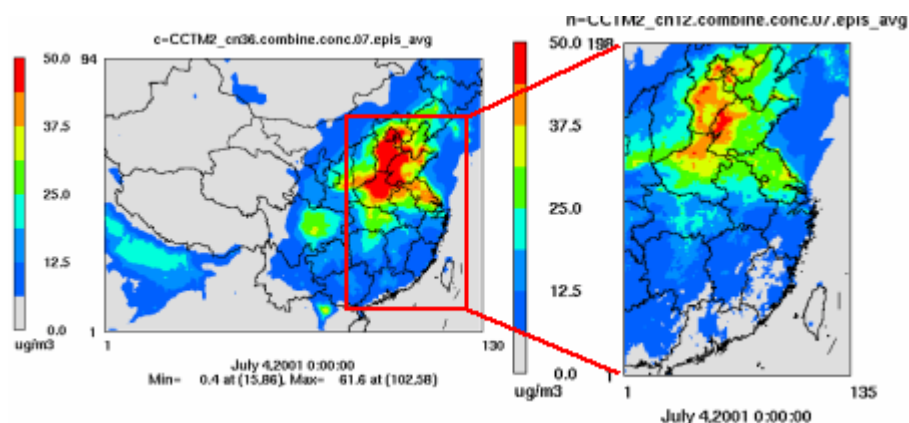
**Figure 9.** Ozone concentrations: (a) base case, (b) 50% increased, (c) 50% reduction



**Figure 10.** PM2.5 concentrations: (a) base case, (b) 50% increased, (c) 50% reduction



**Figure 11.** Visibility concentrations: (a) base case, (b) 50% increased, (c) 50% reduction



**Figure 12.** PM 2.5 episode average in July 2001

research & management tool for regional/urban AQ assessment over China region. We are conducting in 4-km domain in Beijing and Shanghai and are replacing TRACE-P by local emission inventory for the 4-km domain modeling. We will expect more reasonable results.

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