Modeling and Processing Ammonia Emissions for Particulate Matter Studies in the Lower Fraser Valley

Éric Giroux, Helmut Roth, Dazhong Yin, and Weimin Jiang
National Research Council, 1200 Montreal Road, Ottawa, ON, Canada K1A 0R6
eric.giroux@nrc.ca

ABSTRACT

We used the Models-3 Emission Processing and Projection System (MEPPS) to model and process emissions for particulate matter studies in the Lower Fraser Valley of British Columbia, Canada. An issue of interest in the region is the ammonia emission and its impact on the formation of fine particles. The ammonia emissions in the region originate mostly from significant agricultural livestock, with some contributions from other sources such as wastewater treatment and transportation. We identified and corrected two shortcomings of the MEPPS system with respect to modeling and processing ammonia emissions. Firstly, spatial allocation of all area source emissions, including those from agriculture and farming areas emitting large quantities of ammonia, is computed by MEPPS using population and housing surrogates. Secondly, no ammonia emissions result from the modeling and processing of mobile emissions with the underlying MOBILE5a emission factor model.

Due to the structure of MEPPS, it is difficult to use surrogates other than population and housing for spatially allocating area sources. The result is that all the emissions, including ammonia from farming and agricultural areas, are being allocated to centers of population. To correct this problem, we obtained and integrated more detailed spatial surrogate information, and used the alternative Sparse Matrix Operator Kernel Emissions Modeling System (SMOKE) to process the area sources. The ammonia emissions from area sources were clearly shifted from populated centers to the farming and agricultural areas in our modeling domain, giving a more reasonable representation of the reality.

To overcome the lack of ammonia emission factors in MOBILE5a, we obtained ammonia emission factors from the literature for each of the eight vehicle classes used in the system. We combined these factors with the temporally allocated vehicle-miles-traveled in the transportation inventory, and then added the ammonia emissions to other emissions modeled by MEPPS. The contribution of mobile sources to ammonia turned out to be insignificant relative to other ammonia sources in the domain and period of interest in this study.

Based on the improved emission data, the results generated by the Community Multiscale Air Quality (CMAQ) model showed realistic gas phase ammonia and aerosol phase ammonium distributions in the modeling domain.

INTRODUCTION

Under a research project funded by the interdepartmental Program of Energy Research and Development (PERD) in Canada, the National Research Council of Canada is applying a modeling tool for simulating the formation of atmospheric particulate matter. The project is the modeling component of a comprehensive PERD program studying the particulate matter formed by transportation-related sources with coordinated research activities in particle emissions, ambient measurement, computer modeling, and health effects. Part of this modeling project consisted of developing an emissions data set comprised of point, area, mobile, and biogenic sources for input to the CMAQ chemical transport model. This input emissions data set was prepared with the Models-3 Meteorology-Chemistry Interface

Processor (MCIP), MEPPS, the Emission-Chemistry Interface Processor (ECIP), and later modified with SMOKE.

An issue of particular interest in the Lower Fraser Valley is the ammonia (NH_3) emission and its impact on the formation of fine particles. The NH_3 emissions in the region originate mostly from significant agricultural livestock, with some contributions from other sources such as wastewater treatment and transportation.

In the current work, we processed and compared the spatial distribution of Canadian agricultural area source NH_3 emissions by two different sets of spatial surrogates. The first set consisted of population surrogates, while the second set consisted of fertilizer and farm animals surrogates. We also looked at the contribution of mobile sources to the total NH_3 emissions in the domain and period of interest. Lastly, we investigated the effect of these changes on results from CMAQ.

METHODOLOGY

The main software systems used for this project are MEPPS version 3.0, included in the June 1999 release of the Models-3 Framework, and SMOKE version 1.3. They were installed on a Sun Ultra 10 Workstation running Solaris 2.6. As per the MEPPS software requirements, we also installed BASE SAS version 6.12, and ArcInfo version 7.2.1. To visualize the modeling results, we used the Package for Analysis and Visualization of Environmental data (PAVE), version 1.7.1.

The Lower Fraser Valley Modeling Domains

The Horizontal Coordinate System

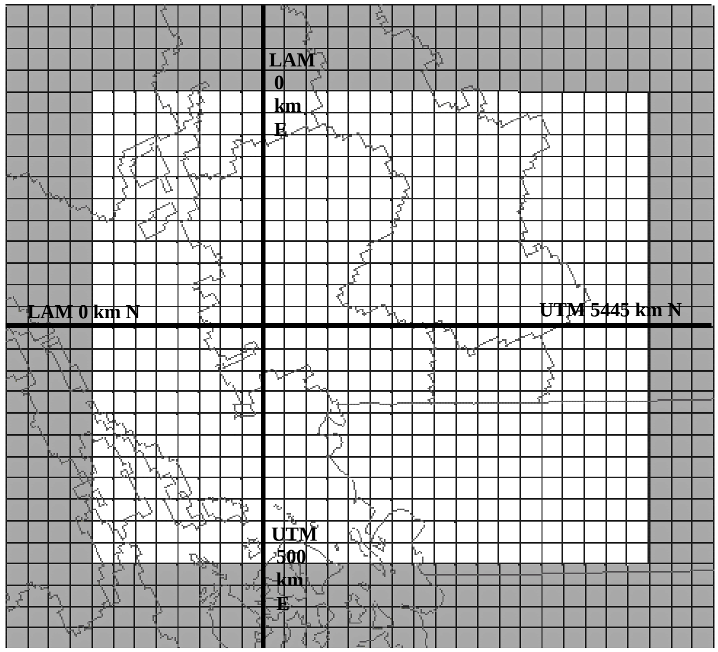
Models-3 requires that the modeling grids be on a Lambert Conformal projection. However, the Pacific '93 emissions inventory[1, 2], which we used in our work, contains some gridded data on a Universal Transverse Mercator (UTM) (zone 10) 5 km mesh, which we refer to as the UTM domain. This domain extends from UTM coordinates (460 km E, 5390 km N) in the southwest to (590 km E, 5500 km N) in the northeast. Several earlier studies[3,4,5,6,7] also used the UTM domain. To be able to directly use the gridded data in the inventory, and to facilitate direct comparison with earlier studies, we chose Lambert projection parameters such that our Lambert grid would closely approximate the UTM grid. Both grids are shown in Figure 1.

The parameters of the Lambert projection are given in Table 1. With these parameters, the coordinate line y = 0 on the Lambert grid coincides with the UTM coordinate line y = 5445 km N, and the Lambert coordinate line x = 0 coincides with the UTM coordinate line x = 500 km E, which in turn coincides with the 123° W meridian. These lines are grid cell boundaries on both the UTM domain and on our CMAQ modeling domains.

Table 1. Lambert conformal projection parameters.

ë$_0$	123°.00
ö$_0$	49°.159782
ö$_1$	48°.75
ö$_2$	49°.50

Figure 1. UTM domain (light) on Lambert inner domain (dark). County boundaries in background.



<u>The Horizontal Grid Domains</u>

The nested inner and outer domains are shown in Figure 2. The inner domain was chosen to include the UTM domain, described above, and shown in Figure 1. Since the inner domain was also to be nested within an outer domain having 15 km grid cells, we collocated boundaries of the inner domain with outer domain grid cell boundaries. The outer domain was to be sufficiently large to properly nest the inner domain for CMAQ runs, and we extended it far enough south to include the urban area of Portland and the Cascadia domain used by Barna and Lamb[8]. This resulted in a 15 km grid extending easterly from –150 km to 225 km (a distance of 375 km, or 25 grid cells), and northerly from -540 km to 120 km (660 km, or 44 grid cells).

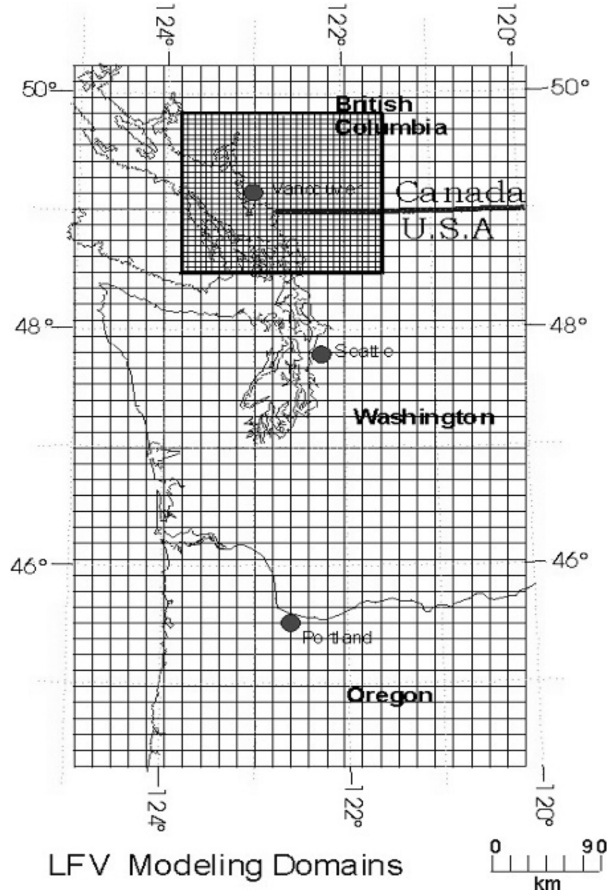
Input Files

Before processing the emissions in MEPPS and SMOKE, it was necessary to setup the Models-3 studies, and to define the grids, vertical layers, and episode. We set up two studies: one for the outer domain, with grids at a 15 km resolution, and one for the inner domain, with grids at a 5-km resolution. These grids are related to the grids used for the Fifth-Generation NCAR / Penn State Mesoscale Model (MM5) model runs[9]. We defined our Lambert projection in the Models-3 Science Manager, and defined the hierarchy of MM5 grids on this projection. This MM5 hierarchy consists of three nested grids with grid cell resolutions of 45, 15, and 5 km, respectively. We defined the episode to run from 1993 July 31 0:00:00 to 1993 August 7 24:00:00, PDT.

<u>Meteorology</u>

Meteorological information was required to model the mobile emissions in MEPPS. This meteorological information comes from the output of MM5 and is processed in MCIP, which vertically interpolates and horizontally subsets the meteorological information and writes files to be used as inputs to MEPPS and SMOKE. We used MM5 version 3 to simulate the meteorology[9] and converted the output files to MM5 version 2 as required by MCIP.

Figure 2. Outer and Inner Domains.



Area Sources Emissions

We used the Environment Canada area source inventories for British Columbia and the Models-3 area source inventories for the states of Washington and Oregon. Both of these inventories are for 1995, and we back cast them to 1993 using a simple population growth model. Population growth data for the United States (US) was obtained from the US census bureau web site, while similar data for the Canadian region was obtained from Levelton Engineering[2].

Spatial allocation in MEPPS uses population and housing surrogates. The Canadian census data provided with Models-3 is at a county level, so to improve accuracy we obtained some approximate enumeration area (census tract) polygons along with their corresponding population and housing data from the Pollution Data Branch at Environment Canada. The approximations, consisting of Thiessen polygons constructed on the true enumeration area centroids, allowed considerable cost savings. The new higher resolution data was then merged with the existing Models-3 data files and GIS coverages.

Due to the structure of the MEPPS system, it is difficult to add and use surrogates other than population and housing for spatially allocating area source emissions. The result is that all the area source emissions, including NH_3 from farming and agricultural areas, are allocated to areas of high population. Somewhat ironically, this problem is exacerbated by the use of the higher resolution population and housing data. To correct the problem, we obtained gridded spatial surrogate information in the Pacific ’93 inventory[1,2] from Environment Canada, Pacific and Yukon Region, and used SMOKE instead of MEPPS to process the Canadian area sources. In one branch of the processing, Canadian emissions from the Source Classification Codes (SCC) listed in Table 2 were allocated by population. In a second branch they were allocated by the improved surrogates: The first SCC in Table 2 was assigned a surrogate profile for fertilizer, while the remaining were assigned a profile for farm animals.

Table 2. SCC codes in the area sources inventory for which we obtained other spatial surrogate information.

SCC	Description
2801700000	Fertilizer application
2805000000	Agriculture – Livestock
2805001000	Beef Cattle Feedlots
2805005000	Poultry Operations
2805015000	Hog Operations

SMOKE expects surrogate ratios normalized over counties. However, the Pacific '93 inventory is domain-specific rather than county-based. The surrogate ratios are thus normalized for the domain rather than for individual counties. Accordingly, we mapped the UTM domain grid cells to counties and then renormalized the ratios for each county.

To process the area source emissions with SMOKE, we first created a surrogate ratios file. We began with the surrogate ratios for population for the entire domain, obtaining these from the MEPPS area source processor, and appended the renormalized, county-mapped Pacific '93 ratios for fertilizer and farm animals. We then generated two SCC-to-Spatial Surrogate Code (SSC) cross-reference files: One in which all sources were referenced to population, and one in which the sources in Table 2 were referenced to the new surrogates.

Smoke runs with these two SCC-SSC cross-reference files then gave us two sets of Canadian area source emissions. These were both merged with the US area sources and the domain wide point and biogenic sources, all of which had already been processed through MEPPS, and the two resulting data sets were later merged with mobile source emissions as described below.

Mobile Sources Emissions

We modeled hourly mobile emissions rates in MEPPS using the mobile-source emission processor. The processor uses a combination of air temperature data at 1.5 m above the surface, mobile source emission factors (computed by the MOBILE5a and PART5 models), fleet vehicle type composition, road types, and Vehicle-Miles-Traveled (VMT).

We obtained a Canadian VMT inventory for the year 1995 from Environment Canada, and used the default 1995 National Emission Trends (NET) inventory included in Models-3 for the US VMT. Both VMT inventories were back cast to 1993 by using regional VMT growth data given by Levelton Engineering[2], and interpolating linearly between 1990 and 1995.

A digital road network was required to spatially allocate VMT data to individual grid cells. The June 1999 release of Models-3 includes a comprehensive Geographical Information System (GIS) database that includes road network coverages for the US, but none for Canada. We acquired a detailed digital road network for our modeling domain. The file was manipulated and merged with the US road network to create a single file suitable for spatial allocation in MEPPS.

The output of the MEPPS mobile-source emission processor is hourly, gridded, and speciated mobile emissions in moles/s. NH_3 is not modeled by the mobile-source emission processor as an emitted contaminant. After investigating with the Criteria Air Contaminants Division of the Pollution Data Branch at Environment Canada, we obtained NH_3 emission factors based on recent research and newer estimation methodologies for NH_3 emission factors[10]. The published NH_3 emission factors for the standard eight vehicle classes of on-road vehicles are presented in Table 3.

Table 3. NH_3 emission factors.

Vehicle Type	NH_3 Emission Factor (g/km)
HDDV	0.00193
HDGT	0.02992
LDDT	0.00193
LDDV	0.00193
LDGT	0.07572
LDGV	0.07200
MC	0.00109

To calculate NH_3 emissions, we first extracted the spatially- and temporally-allocated VMT from MEPPS intermediate processing files. The emission factors in Table 3 were then combined with the VMT to obtain NH_3 emissions, and emissions from all eight vehicle classes were aggregated together. The resulting NH_3 emissions were merged with the other mobile emissions to generate a single new mobile source emissions file.

Finally, the original (no NH_3) motor vehicle emissions were merged with the emissions data containing Canadian area sources allocated by population, and the new motor vehicle emissions (with NH_3) were merged with the emissions data containing the reallocated Canadian area sources. Both data sets were then used as input to CMAQ.

RESULTS

This section presents the results of our modeling work with MEPPS, SMOKE and CMAQ. The CMAQ outer domain run was used to generate initial and boundary conditions for the inner domain runs. The inner domain is the domain of interest and we present results for that domain only.

Table 4 shows the average grid cell emission rate for NH_3, the average being taken over all time steps and grid cells. The percentage contribution from area, mobile, and point sources is given. There are no contributions from biogenic sources. We note that area sources are overwhelmingly (99.7%) responsible for the NH_3 emissions.

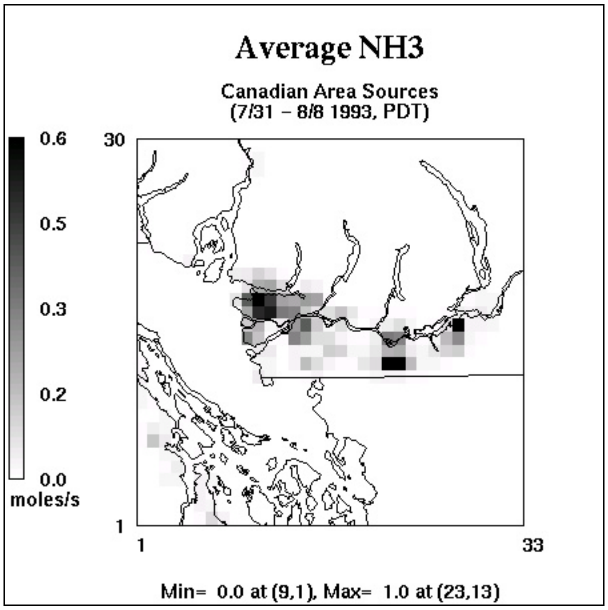
Table 4. NH_3 contributions from area, mobile, and point sources.

	Episode-averaged NH_3			
NH_3 statistic	**All sources**	**Area**	**Mobile**	**Point**
cell average (µmoles/s)	23488	23412	1.7	73
cell average (%)	100.0	99.68	0.01	0.31

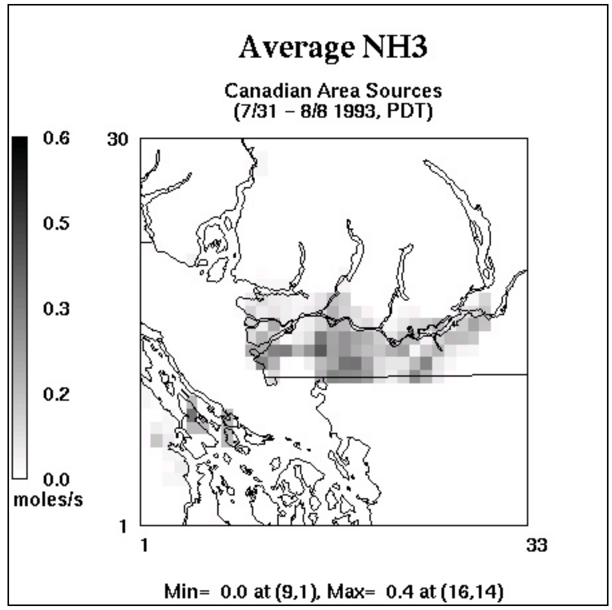
Distribution of NH_3 Emissions from Area Sources

Figure 3 depicts the spatial distribution of the episode-averaged NH_3 emissions from Canadian area sources. In Figure 3a we see the distribution of area source emissions allocated using the population surrogates, while Figure 3b shows the improved spatial distribution resulting from the use of the fertilizer and farm animals surrogates for the allocation of the five SCCs listed in Table 2.

Figure 3. Spatial distribution of episode-averaged Canadian area source NH_3 emissions. (a) Original spatial allocation by population surrogate ratios. (b) Improved spatial allocation of farming-related activities.



(a)



(b)

In the Canadian part of the domain, it is clear from Figure 3a that the spatial allocation using population surrogate ratios for all area sources resulted in the emissions being allocated to highly populated areas. We note that there are four high NH_3 centers in this figure. They are, from left to right, the cities of Vancouver, Surrey, Abbotsford and Chilliwack.

The improved spatial allocation of the NH_3 emissions shown in Figure 3b resulted in the emissions being shifted away from all of the four city locations mentioned above, and re-allocated over the agricultural areas.

Contribution to NH_3 emissions by Mobile Sources

As shown in Table 4, the mobile sources contribution to the total NH_3 emissions is insignificant. The large contribution to NH_3 emissions from livestock production overwhelms both the point source and mobile contributions. The spatial distribution of the episode time averaged mobile source NH_3 emission rate over the inner domain is shown in Figure 4.

Effect of the Modified Emissions on the CMAQ Ammonia and Ammonium Concentration Fields

Our outer domain CMAQ run used an emission data set generated by MEPPS with no further modifications. For the inner domain, we ran CMAQ with the two emissions data sets described above. All other inputs to the model were left unchanged.

Figure 4. Episode-averaged NH_3 emissions from mobile sources.

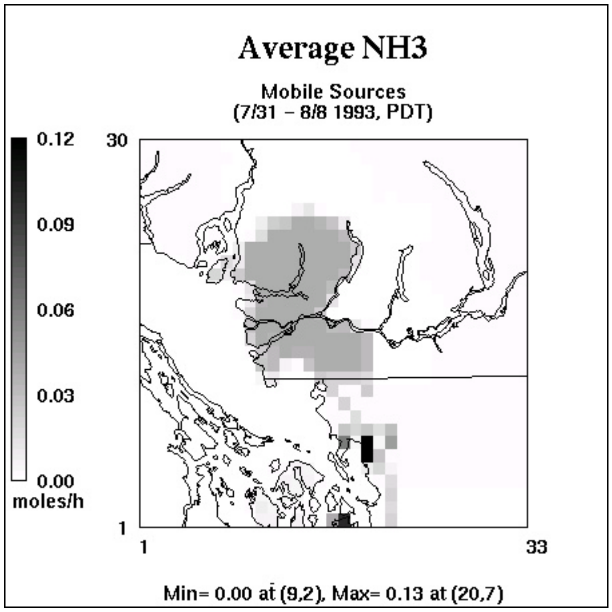
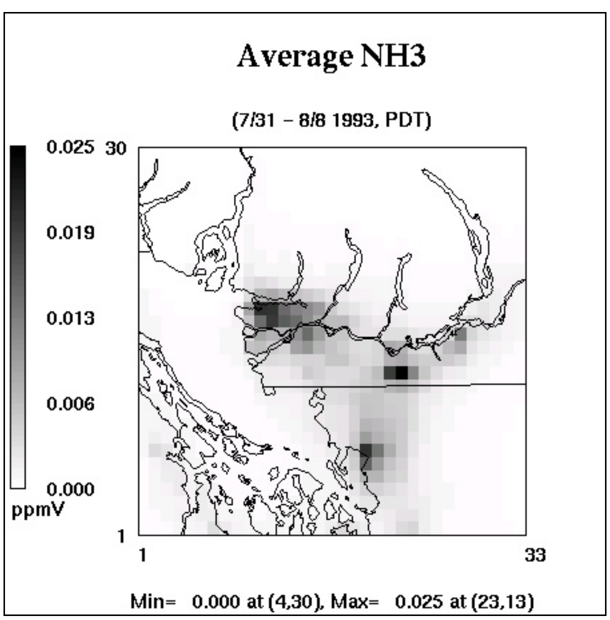
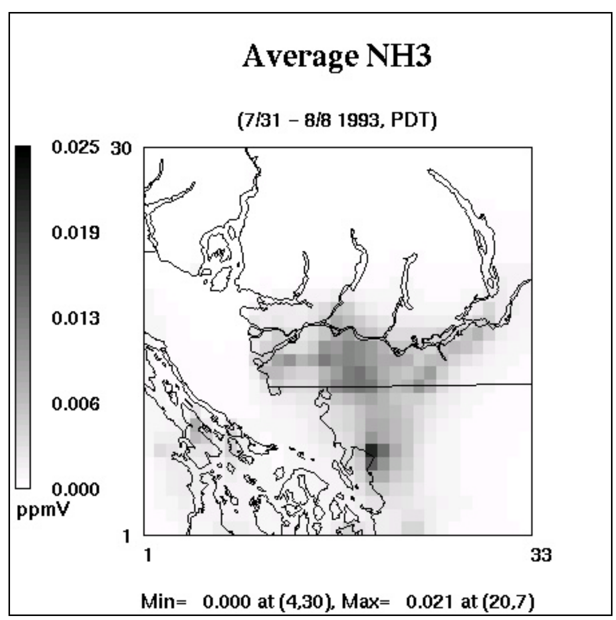


Figure 5 depicts the episode-averaged NH_3 concentration field in the first vertical layer. In Figure 5a, NH_3 is concentrated in highly populated areas with 3 major centers: Vancouver and Abbotsford in Canada, and the city of Bellingham in the US. In Figure 5b, NH_3 is now shifted to the agricultural areas in the Canadian part of the domain, while no change occurred in the US. The US area source emissions were allocated by MEPPS using population and housing surrogate ratios in both cases. This serves as a comparison to see the impact of modifying the spatial surrogates. We will modify this later for our final model runs.

Figure 5. Spatial distribution of the episode-averaged NH_3 concentration field modeled by CMAQ. The emissions input to CMAQ were generated using: (a) Original spatial allocation of Canadian area sources by population surrogate ratios. (b) Improved spatial allocation of the farming-related activities in Canada.



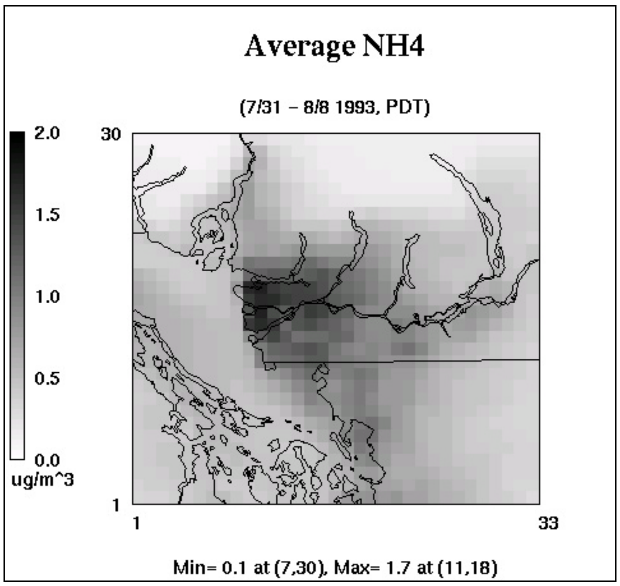
(a)



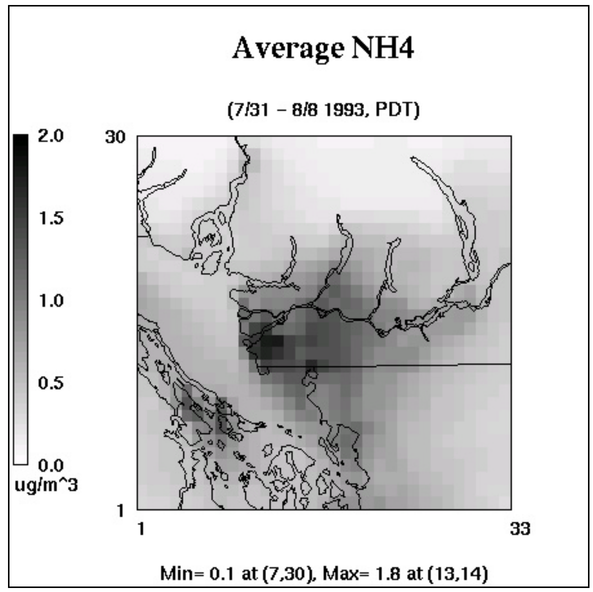
(b)

The spatial distribution of episode-averaged aerosol-phase ammonium (NH_4) is presented in Figure 6. Again, the spatial patterns indicate a southerly shift of high NH_4 concentration from populated areas (notably Vancouver – Figure 6a) towards farming and agricultural areas (Figure 6b).

Figure 6. Spatial distribution of the episode-averaged NH_4 concentration field modeled by CMAQ. The emissions input to CMAQ were generated using: (a) Original spatial allocation of Canadian area sources by population surrogate ratios. (b) Improved spatial allocation of the farming-related activities in Canada.



(a)



(b)

CONCLUSIONS

Spatial allocation of agricultural NH_3 emissions with surrogates related to agriculture rather than population shifted the emissions from regions of relatively high population density to regions of agricultural activity, resulting in a more reasonable distribution of emissions.

The mobile sources contributed negligibly to the total NH_3 emissions in the domain/episode of interest. NH_3 emissions in this study were dominated by agricultural area source emissions.

Based on the improved emission data, the results generated by CMAQ showed realistic ammonia and ammonium distributions in the Canadian part of our modeling domain. The observed redistribution clearly indicates the need for appropriate surrogate data sets and the tools to use them easily.

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KEYWORDS

Area Sources
Ammonia
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Lower Fraser Valley
MEPPS
Mobile Sources
Models-3
SMOKE
Spatial Surrogates
Spatial Allocation