Surrogate Selection within SMOKE to Obtain Realistic Spatially Resolved Mobile Source Emissions

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ABSTRACT

Emission preprocessing, defined as the creation of a spatially and temporally resolved emissions inventory from raw data, is a crucial part of air quality modeling. We have focused on improving emission preprocessing using the SMOKE system. Because emissions are rarely distributed evenly with respect to location, gridding surrogates are used to apportion emissions to each grid within the modeling domain. New gridding surrogates with a 4 km x 4 km grid resolution for the eastern United States, developed by the state of New York, have recently become available. Previously, emissions from on-road mobile sources have been distributed using urban area and rural area surrogates. The new surrogate accounts for the location of major highways, and use of this new surrogate is expected to produce a more reasonable distribution of emissions from on-road mobile sources.

To investigate the impact of the choice of surrogate on emission distributions, we made incremental changes to the surrogate assignments for on-road mobile sources, changing from either urban area or rural area to the new surrogates which include major highways. The results of the SMOKE emissions inventory simulations for the state of Maryland performed for the test day of July 1, 1996 showed significant differences. These results suggest that the choice of gridding surrogate has a significant effect on both the spatial distribution and local magnitude of the predicted emissions. Thus, careful assignment of appropriate surrogates to each source is an important step towards developing a more reasonable and representative emissions inventory.

INTRODUCTION

Air quality modeling has been used to simulate the complex physical and chemical processes in the atmosphere. Model simulations are needed to identify the sources of a problem, contributing factors, and methods for controlling or alleviating pollutant emissions, in order to understand the causes of air pollution and effective means of reduction. Typically, an air quality model would be used to simulate a variety of alternative scenarios in a comparative manner to help the regulatory user arrive at appropriate control strategies. Therefore, accurate processing as well as the use of appropriate data in modeling is essential for defining appropriate control strategies.

Emission models, one of main components of an air quality modeling system, with meteorology, chemistry and transport, are used to make input files ready for air quality prediction. Our main goal is to improve the accuracy of emissions preprocessing strategies, as a part of a larger air quality modeling and measurements program. In this study, Sparse Matrix Operation Kernel Emissions (SMOKE), an emission pre-processing model developed by North Carolina Supercomputing Center (NCSC), is employed to study the effect of the choice of surrogate in the gridding step on the output of SMOKE.

SMOKE PROCESSING

SMOKE is used to convert the source-level emissions (tons per year per county per source) to gridded, speciated, and temporally processed emissions (tons per hour per grid cell per source). This conversion consists of multiplying emissions of various sources by several factors in steps called temporalization, speciation, and gridding.

At each step, the processing model uses profile tables and cross-reference tables to convert or modify the emission resolution. The profile tables contain the factors for converting emissions from county wide, yearly emissions to hourly emissions with finer spatial resolution. Cross-reference tables are used to assign the profiles to each source.[1]

In the temporalization step, SMOKE creates an hourly pollutant emissions inventory by applying the monthly, weekly, and diurnal profiles based on the source characteristics, using the cross-reference table to match the profile to the source type. In the speciation step, it creates a speciation matrix containing conversion factors, used to convert Volatile Organic Compound (VOC) concentrations to the concentrations of specific organic compounds. There are nine specific organic compounds for the Carbon-Bond IV (CB4) chemical mechanism. The CB4 mechanism is one of many mechanisms developed to represent chemical interactions among atmospheric constituents. This lumped structure mechanism creates a balance between computing efficiency, which favors compressed chemical mechanisms, and accuracy, which demands explicit treatment of chemical reactions, and favors large chemical mechanisms.[2] The nine organic compounds for the partitioning of VOC are ethene (ETH), isoprene (ISOP), formaldehyde (FORM), paraffin (PAR) representing single carbon bonds, olefin (OLE) representing double-bonded carbon atoms, toluene (TOL) representing 7-carbon ring structures, xylene (XYL) representing 8-carbon ring structures, acetaldehyde (ALD2) representing carbonyl group and adjacent carbon atoms in acetaldehyde and higher molecular weight aldehydes, and non-reactive carbon atoms (NR).[3] In the gridding or spatial allocation step, SMOKE uses a gridding surrogate to create a matrix containing conversion factors, used to transform county level aggregate emissions to emissions in each grid cell. A gridding surrogate is a dataset developed from geographic information (e.g. population or land use) at a finer spatial resolution than the initial emissions data, and it is used to spatially allocate the emissions to the grid cells.[4]

EFFECT OF SURROGATE SELECTION WITHIN SMOKE

We obtained new gridding surrogates with a 4 km x 4 km grid resolution for the eastern United States, recently developed by the state of New York.[5] The new surrogates include one based upon the locations of major highways. We expected that the use of the surrogate, major highways, for on-road mobile sources would distribute emissions more appropriately than the use of urban and rural surrogates. To investigate the effect of surrogate selection, an on-road mobile emissions inventory for 1996 for the state of Maryland, provided by the Maryland Department of the Environment, was used.

The first step towards using the new surrogate was to modify the gridding cross-reference table, which assigns a surrogate to each source, for the on-road mobile sources.

We made incremental changes to the surrogate assignments for on-road mobile source types, changing from either urban area or rural area to the major highways surrogate. On-road mobile sources are categorized by both vehicle and road type. The last three digits of the Standard Classification Code (SCC) denote the road type. There are 12 road types in the SCC: Rural Interstate (RI), Rural Principal Arterial (RPA), Rural Minor Arterial (RMA), Rural Major Collector (RMC), Rural Minor Collector (RMIC), Rural Local (RL), Urban Interstate (UI), Urban Freeway (UF), Urban Principal Arterial (UPA), Urban Minor Arterial (UMA), Urban Collector (UC), and Urban Local (UL).

As Table 1 shows, we considered five different surrogate assignments, starting from the base case. In addition, Change No. 4 was studied to determine what differences would result when the population surrogate for rural and urban local roads was assigned instead of the rural area and urban area surrogates.

Table 1. Five different changes to the assignments of surrogates

	Urban/Rural surrogates	Major highways surrogates	Population surrogates
Base Case	All road types		
Change No. 1	RMA, RMC, RMIC, RL, UMA, UC, UL	RI, RPA, UI, UF, UPA	
Change No. 2	RL, UL	RI, RPA, RMA, RMC, RMIC, UI, UF, UPA, UMA, UC	
Change No. 3		All road types	
Change No. 4		RI, RPA, RMA, RMC, RMIC, UI, UF, UPA, UMA, UC	RL, UL

We performed simulations for the state of Maryland for the test day of July 1, 1996. Figures 1, 2, 3, 4, and 5 show the distributions of CO emissions at 3 pm for each change. The maximum CO emission rate, predicted using the original surrogate assignments (Base Case), occurred at a location in Baltimore County (grid cell # : (63, 48)), at a rate of 0.651 tons/hr. However, the maximum CO emission rates, predicted using the new surrogate (Change No. 1, 2, 3, and 4), were observed at a location within the city of Baltimore (grid cell # : (65, 47)), at rates of 0.857, 1.188, 1.293 and 1.275 tons/hr for the same time of day, respectively. Similar results were observed for both NOx and VOC emissions.

Figures 6, 7 and 8 show the difference in emission rate of CO, NOx, and VOC that occurs when Change No. 4 is applied, rather than the Base Case. Significant differences in concentrations of all three pollutants are observed in most of Montgomery County, and Prince Georges County.

CONCLUSIONS

This study suggests that the choices of gridding surrogate can lead to different results in mobile source emission allocations because gridding surrogate selection significantly affects both the spatial distribution and local magnitude of the predicted emissions. Hence, in order to insure a reasonable and appropriate emissions inventory for developing control strategies, careful assignment of appropriate surrogates to each source should be performed.

ACKNOWLEDGEMENTS

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4. Choi, Y.J; Mitchell, M.; Barnes, T.; Ehrman, S.H.; Calabrese, R.V., “Towards improved emission preprocessing using SMOKE”, *In proceedings, 94th Annual meeting of the Air and waste Management Association*, Orlando, Florida, 2001; Paper #188.
5. New gridding surrogate download site: http://envpro.ncsc.org/emcenter/

KEYWORDS

SMOKE, Selection of Gridding Surrogate, Emission Preprocessing

Figure 1. Distribution of CO emissions for Base Case

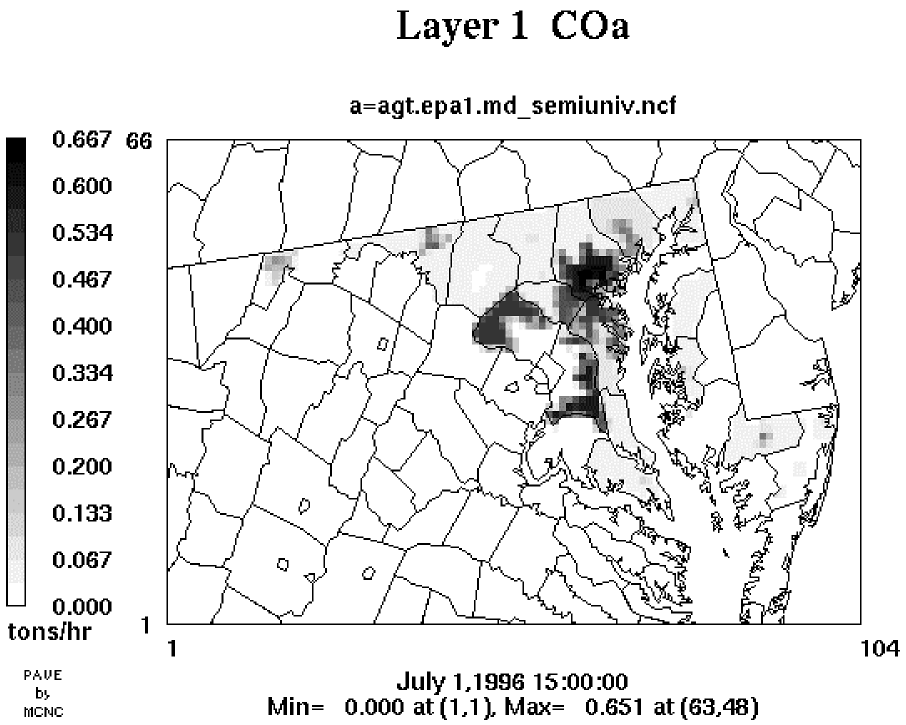

Figure 2. Distribution of CO emissions when Change No.1 to surrogates is applied

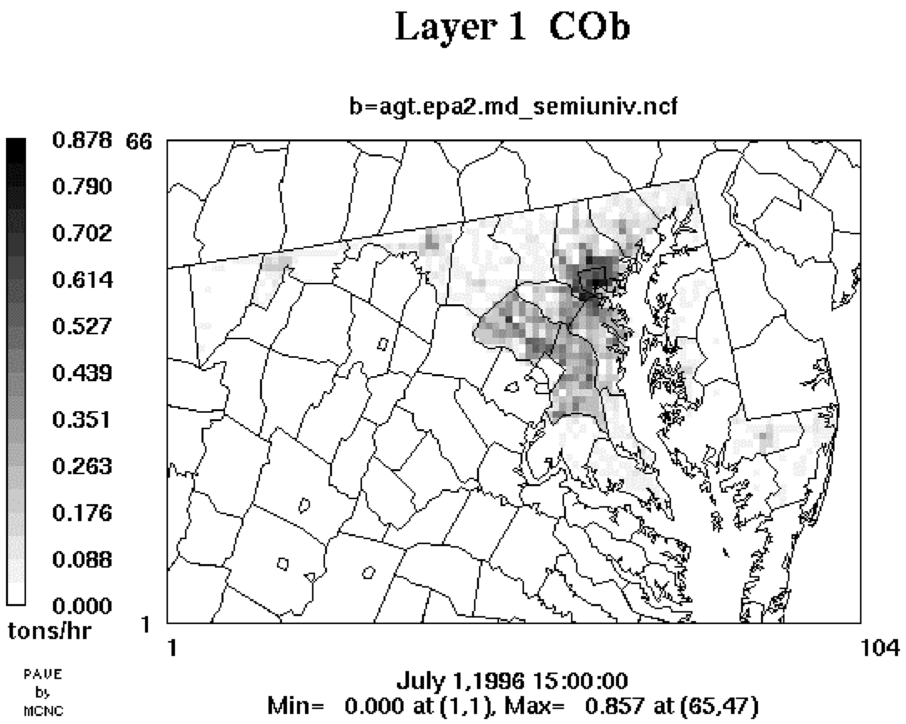

Figure 3. Distribution of CO emissions when Change No.2 to surrogates is applied

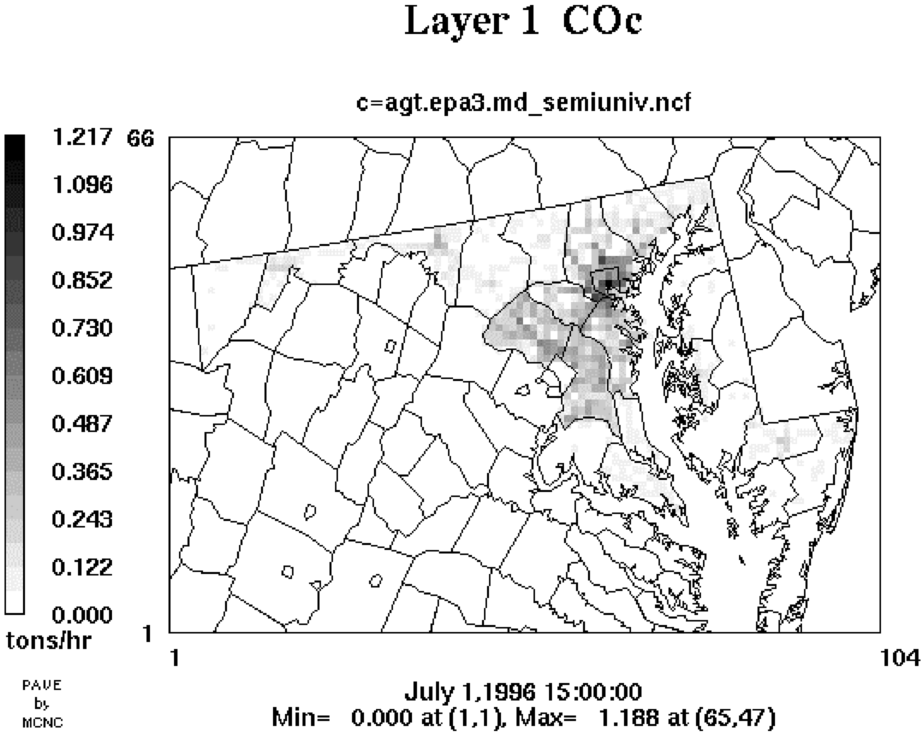

Figure 4. Distribution of CO emissions when Change No.3 to surrogates is applied

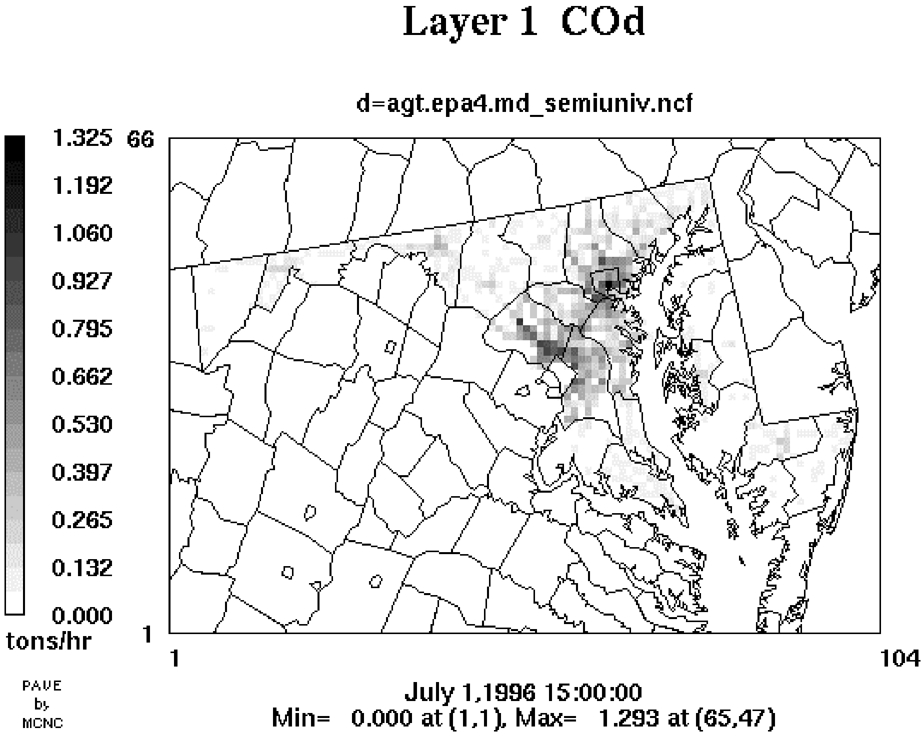

Figure 5. Distribution of CO emissions when Change No.4 to surrogates is applied

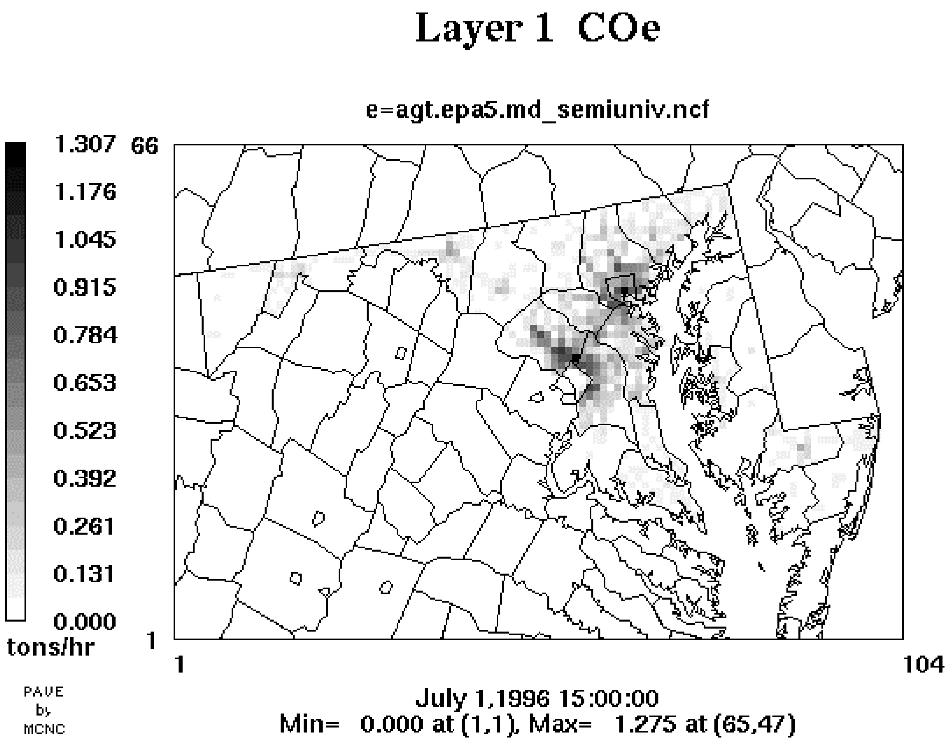

Figure 6. Difference between the CO emissions generated using the Base Case, and that generated using Change No. 4

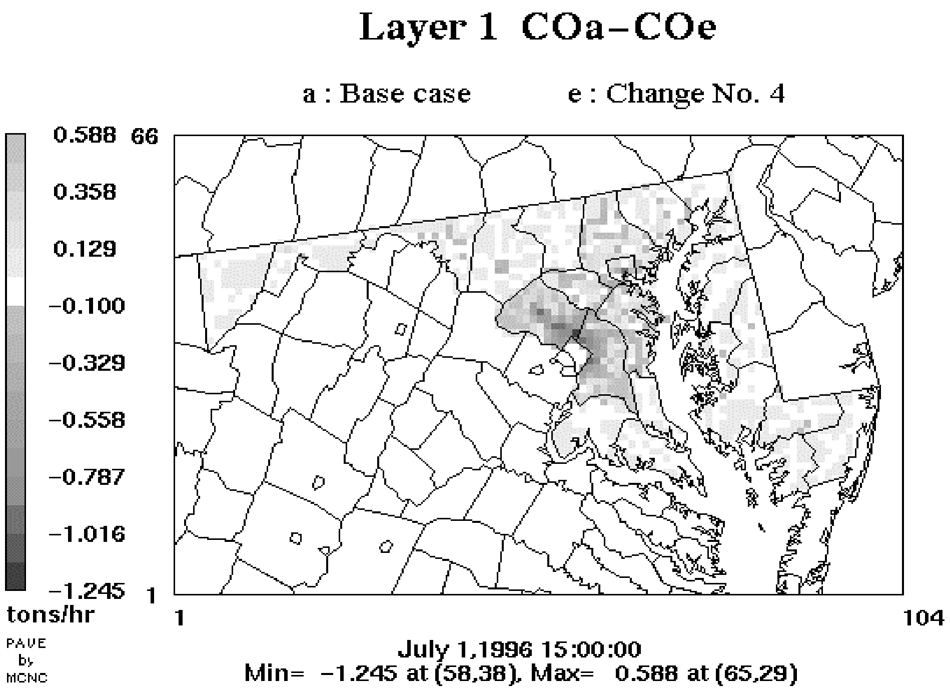

Figure 7. Difference between the NOx emissions generated using the Base Case, and that generated using Change No. 4

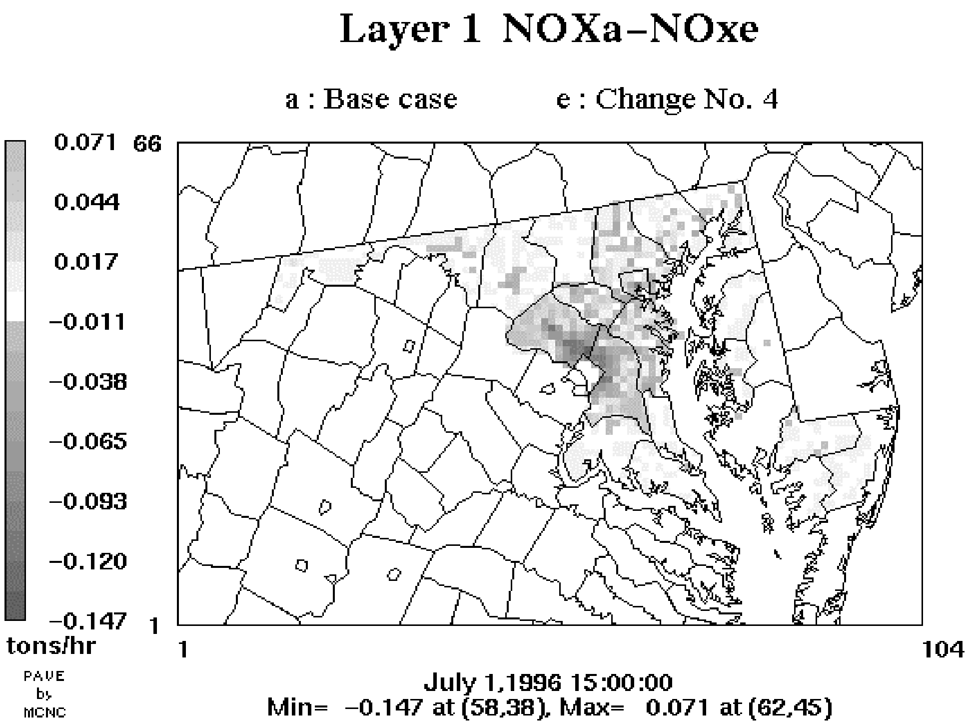

Figure 8. Difference between the VOC emissions generated using the Base Case, and that generated using Change No. 4