

## EMISSIONS INVENTORY DEVELOPMENT FOR FINE-SCALE AIR QUALITY MODELING

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### \* 1. INTRODUCTION

In the air quality modeling community, photochemical grid models are generally run for horizontal grid resolutions of 36 km and 12 km; however, increasing attention is being given to resolving pollutant concentrations at finer spatial scales in response to a variety of air quality management issues.

For example, because modeling at a 12-km resolution may not adequately capture local source impacts on ambient PM<sub>2.5</sub> concentrations at Federal Reference Method (FRM) monitoring sites, EPA guidance on the use of models for National Ambient Air Quality Standards (NAAQS) attainment demonstrations includes a discussion on the use of dispersion models for "local area analysis" in areas with large spatial gradients of primary PM<sub>2.5</sub> (U.S. Environmental Protection Agency, 2007).

As a result, many state and local agencies are now conducting local area analyses and performing fine-scale air quality modeling for State Implementation Plan (SIP) attainment demonstrations. Such efforts require the development of local-scale emissions inventories that are more representative of individual facilities and other local sources than information contained in the National Emissions Inventory (NEI), EPA's AP-42 emission factor compendium, and other inventory "building blocks."

In addition to PM<sub>2.5</sub> attainment issues, fine-scale concentration gradients are of concern for air toxics evaluations, which exhibit areas of high concentration near emissions sources such as roadways (Cook et al., 2008). Because both air toxics and criteria pollutants require local-scale evaluations, there is greater need to provide multi-pollutant and multi-scale air quality information. As a result, EPA's Office of Air Quality Planning

and Standards (OAQPS) recently conducted a pilot study in Detroit, Michigan, to develop and undertake multi-pollutant, risk-based analyses. The Detroit study approach featured hybrid air quality modeling that combined regional modeling at a 12-km grid resolution with urban-scale dispersion modeling at a 1-km resolution. This hybrid approach was designed to account for the contribution of local sources to PM<sub>2.5</sub> and air toxics concentrations in the Detroit area (Tooly and Wesson, 2009).

To build capacity in EPA's Emissions Inventory and Analysis Group (EIAG) and the state, local, regional, and tribal (SLRT) inventory community for local-scale emissions inventory evaluation and improvement techniques, EPA staff formed a focus group from state and local agencies that are developing local-scale inventories for fine-scale modeling. The objectives of this project were to

- Determine the types of inventory data analyses that can assist SLRT agencies with local-scale inventory development.
- Prioritize beneficial analyses and recommend how they might be systematically applied to the EPA's NEI and distributed as data and/or results.
- Assess the availability of local-scale emissions data and how these data are related to data in the EPA's Emission Inventory System (EIS) and to the NEI data collection process.

Sonoma Technology, Inc. (STI) provided support to EPA by helping facilitate teleconferences, reviewing technical documentation provided by state and local agencies, and documenting project findings.

### 2. TECHNICAL APPROACH

At the outset of this project, EPA staff identified SLRT agencies that are developing local-scale inventories for fine-scale modeling and

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recruited representatives from these agencies to participate in the local-scale emissions inventory focus group. During this process, two types of focus group participants were recruited: (1) core participants who would present information on local-scale analyses performed by their agencies; and (2) peer reviewers who would participate in group meetings and review group work products. **Table 1** provides a list of participating agencies and summarizes the types of local-scale analyses conducted by core participants' agencies.

Table 1. List of local-scale emissions inventory focus group participants.

Agency	Purpose of Local-Scale Analyses
<b>Core Participants</b>	
Allegheny County (PA) Health Department	Evaluation of local emissions contributing to monitored PM <sub>2.5</sub> levels
Alabama Department of Environmental Management	SIP attainment demonstrations for ozone and PM <sub>2.5</sub>
Cleveland Division of Air Quality	Multi-pollutant study (PM <sub>2.5</sub> and air toxics)
Georgia Department of Natural Resources	PM <sub>2.5</sub> attainment demonstration for Atlanta
Illinois Environmental Protection Agency	PM <sub>2.5</sub> attainment demonstration for St. Louis
Missouri Department of Natural Resources	See above
Wyoming Department of Environmental Quality	Evaluation of wintertime high ozone episodes associated with oil and gas production
<b>Peer Reviewers and Other Participants</b>	
Indiana Department of Environmental Management	
Pennsylvania Department of Environmental Protection	
Maricopa County (AZ) Air Quality Department	
Maricopa Association of Governments	
Pinal County (AZ) Air Quality Control Division	
Puget Sound (WA) Clean Air Agency	
EPA Region 3	
EPA Region 7	
EPA Region 8	

The focus group met via teleconference on a biweekly basis from May 19 through August 24, 2010. Core participants presented and discussed information related to several charge questions:

- 1) What type of air quality problems were addressed with the fine-scale modeling conducted by state and local agencies?
- 2) What analysis techniques were used to evaluate emission biases, identify key sources in their area, and prioritize emissions inventory improvement work?
- 3) For which source categories were emissions estimates improved, and what methods were used?
- 4) What changes to emissions estimates and modeling results occurred because of local-scale emissions inventory development efforts?
- 5) Would any NEI-related analyses be helpful to their efforts? (If so, at what step in the process would such analyses be beneficial?)

In addition, SLRT agencies provided EPA and STI with technical support documents related to their local-scale inventory development and fine-scale modeling efforts. These documents were reviewed to gain additional insights into issues identified by the charge questions listed above. At the conclusion of the project, EPA and STI summarized the information gathered from SLRT agencies, highlighted patterns in approaches taken and results achieved, and developed recommendations for local-scale inventory development practices and potential NEI analyses that could assist the local-scale inventory development process.

### 3. RESULTS AND DISCUSSION

The sub-sections that follow present and discuss results from the focus group meetings; the project findings are organized by the five charge questions listed above.

#### 3.1 Air Quality Problems Addressed

The Clean Air Act requires that states submit SIPs to demonstrate how EPA-designated "non-attainment" areas (NAAs) for PM<sub>2.5</sub>, ozone, or other pollutants will attain the violated standard(s). Almost exclusively, state and local agencies that participated in the focus group conducted local-scale emissions inventory development and fine-scale modeling as part of SIP attainment

demonstrations or related investigations of local source contributions to pollutant concentrations.

In particular, state and local agencies focused their efforts on local area analyses conducted to address local source primary PM<sub>2.5</sub> contributions to “excess” PM<sub>2.5</sub> concentrations at individual monitoring sites. For example, the Allegheny County Health Department (HD) conducted a local area analysis in the Liberty-Clairton NAA, an area covering only 12 square miles in southeastern Allegheny County. The Liberty-Clairton NAA and its environs are home to several large industrial facilities, including the largest coke plant in the country (Graham and Maranche, 2010).

Similarly, Illinois EPA and the Environmental Protection Division (EPD) of the Georgia Department of Natural Resources (DNR) conducted local area analyses that were driven by localized PM<sub>2.5</sub> exceedances. Illinois EPA’s analysis focused on iron and steel manufacturing in the area around the Granite City monitoring site in the St. Louis PM<sub>2.5</sub> NAA (Sprague, 2010), while Georgia EPD’s work focused on Atlanta’s Fire Station #8 (FS#8) monitor, which exhibits higher annual average PM<sub>2.5</sub> measurements than other monitors in the Atlanta NAA and is located near three large rail yards (Boylan, 2010). Both analyses featured fine-scale dispersion modeling with AERMOD for local sources.

While local sources of primary PM<sub>2.5</sub> were the primary focus of local-scale emissions inventory development and fine-scale modeling by state and local agencies, ozone non-attainment issues also played a role in some cases. For example, the Wyoming Department of Environmental Quality (DEQ) has been evaluating localized ozone exceedances in the Upper Green River Basin (UGRB) that are driven by the rapid growth of oil and gas production activities in the UGRB, as well as the distinct meteorological conditions in this area (e.g., persistent wintertime inversion events with low mixing heights). Wyoming DEQ is working to develop detailed, well-specific emissions inventories for the UGRB and other oil and gas production fields in the state to support ozone modeling efforts (Bohlmann and Rairigh, 2010).

Finally, local-scale emissions inventories are also being developed to support multi-pollutant analyses in urban-areas. For example, as part of the Cleveland Multiple Air Pollutant Study (CMAPS), STI worked with EPA and the Cleveland Division of Air Quality (DAQ) to develop improved emissions inventories for industrial facilities and other sources in Cleveland for use in PM<sub>2.5</sub> and air toxics modeling (Reid et al., 2010).

### 3.2 Analysis Techniques

Among the state and local agencies that participated in the focus group, a variety of analysis techniques were used to evaluate emission biases, identify key sources in areas of interest, and prioritize emissions inventory improvement work. Techniques widely used by the participating agencies include inter-monitor comparisons, meteorological analyses, and receptor modeling with positive matrix factorization (PMF).

For example, Georgia EPD used inter-monitor comparisons during the development of a SIP for the Atlanta NAA. EPD compared long-term trends in PM<sub>2.5</sub> data from three monitoring sites in Atlanta and found that, over time, the FS#8 site consistently recorded PM<sub>2.5</sub> levels substantially higher than were recorded at other Atlanta sites (Georgia Department of Natural Resources, 2010). Similarly, Illinois EPA developed daily average “base concentration” data for eight compliance monitoring stations in the St. Louis area and compared these base values to monitor-specific daily average PM<sub>2.5</sub> concentrations to identify monitoring sites with significant impacts from local sources (Sprague, 2010).

To provide additional insights into local sources that may be impacting monitoring sites, some agencies combined ambient measurements with wind direction data to determine which wind directions were prevalent when high pollutant concentrations were observed. For example, Georgia EPD plotted PM<sub>2.5</sub> concentrations against wind direction data at three monitoring sites in the Atlanta NAA, including the FS#8 site. Results showed that PM<sub>2.5</sub> levels at all three sites were highest when winds were from the south, which was expected, as all three sites lie north of downtown Atlanta. However, PM<sub>2.5</sub> peaks were observed on days of southwesterly winds at the FS#8 site but not at the other two sites. This finding indicated impacts on the FS#8 site from a large rail yard southwest of the site (Georgia Department of Natural Resources, 2010).

State and local agencies also used the PMF receptor model to help identify and quantify impacts from local emissions sources. PMF is a multivariate factor analysis tool used to identify a group of sources that best characterize ambient data at a monitoring site and the amount of mass contributed by each source to measured pollutant concentrations (Norris et al., 2008). Allegheny County HD used PMF to characterize the PM<sub>2.5</sub> increment at the Liberty monitor in Allegheny

County's Liberty-Clairton NAA. The Liberty monitor measures 54 different species of PM<sub>2.5</sub> in addition to the total mass concentration; PMF modeling of the speciated data resulted in the identification of 12 source factors. Apart from secondary ammonium sulfate, the factor with the highest contribution to PM<sub>2.5</sub> mass at the Liberty monitor was the "carbon-rich" factor, which contains high percentages of elemental and organic carbon. The Allegheny County HD estimated that the majority of this factor was contributed by a constant industrial source, most likely a large coke plant that was subsequently prioritized for improved emissions estimation (Maranche, 2006). PMF modeling was also used to investigate local source contributions to measured PM<sub>2.5</sub> concentrations in Atlanta by Georgia EPD (Georgia Department of Natural Resources, 2010), in Birmingham by Alabama DEM (Bacon and Cole, 2010), and in Granite City by Illinois EPA (Sprague, 2010).

Other analyses used to identify key sources in areas of interest included the calculation of emissions-to-distance ratios to evaluate the probability that emissions from individual facilities would contribute to monitored PM<sub>2.5</sub> concentrations. Alabama DEM used emissions rates (Q) and distance-to-monitor data (D) for individual facilities in the Birmingham area to calculate Q/D values for each facility and rank all facilities according to potential impacts on monitoring sites (Bacon and Cole, 2010).

### **3.3 Emissions Inventory Improvement Methods and Outcomes**

Local-scale emissions inventory development efforts undertaken by state and local agencies in support of attainment demonstrations and other analyses focused primarily on large industrial sources such as steel mills. However, non-point sources (e.g., oil and gas production wells), non-road mobile sources (e.g., locomotives at rail yards), and on-road mobile sources were also addressed.

Methods used to improve emissions estimates for industrial facilities included facility surveys, stack testing, and evaluation of stack parameters and other modeling inputs. For example, the Allegheny HD used updated stack testing at a large coke plant to develop new emission factors for condensable and filterable PM<sub>2.5</sub> from the facility's quench towers. These updates resulted in a base-year increase of over 1,700 tons per year for primary PM<sub>2.5</sub> emissions. For CMAPS, STI conducted telephone and email surveys of 21

high-priority facilities in Cleveland and collected information on emissions and operating conditions for the months of August 2009 and February 2010, when intensive air quality monitoring was being conducted. Information gathered through the surveys was used to generate day-specific emissions inventories and account for times when facilities were shut down or had reduced operations (Reid et al., 2010).

Because of the rapid expansion of oil and gas production activities in Wyoming's UGRB and the contribution of these sources to elevated wintertime ozone concentrations, Wyoming DEQ has instituted an extensive minor-source permitting program that covers all oil and gas production wells in the state. Though such wells are typically aggregated in emissions inventories as county-level non-point sources, Wyoming DEQ began collecting "bottom-up" emissions data for all permitted wells in 2009 so that these wells could be treated as individual point sources in air quality modeling applications. These well-specific inventories cover 14 emissions sources, including drill rigs, stationary engines, process burners, tanks, dehydration units, pneumatic pumps, and non-road mobile sources (Bohlmann and Rairigh, 2010).

Non-road mobile sources addressed during local-scale analyses include locomotives operating at rail yards in Atlanta (Boylan, 2010) and commercial marine vessels operating at the Port of Cleveland (Reid et al., 2010). In both cities, individual facilities were contacted to gather information on locomotive activities and vessel calls, respectively.

### **3.4 NEI-Related Analyses**

State and local agencies that participated in the local-scale focus group observed that, while the NEI serves as a good starting point for regional modeling applications, concerns exist regarding the quality and detail of the data with respect to local-scale analyses, specifically, the quality of stack parameter information, location coordinates, temporal resolution, and spatial resolution (e.g., county-level vs. link-based mobile source estimates).

Some focus group time was devoted to discussing the relationship between local-scale inventories and the NEI, and the extent to which emissions inventory improvements made during local area analyses are captured in local data systems and made available to the EPA's EIS. Based on these discussions, there appears to be a lack of connection between local-scale inventories

developed for SIP modeling purposes and state inventories submitted to EPA's EIS for inclusion in the NEI. SLRT agencies that participated in the focus group indicated that, though some of the emission rates, stack parameters, and other local-scale information collected will be included in EIS submittals, a number of barriers exist that hinder this process. Specific barriers identified include

- The timing of inventory updates, which may occur on the heels of a state's EIS submittal.
- The resources required to prepare detailed local-scale emissions inventories (e.g., oil and gas well data) for submittal to the EIS.
- The fact that emissions inventories prepared for local area analyses and SIP modeling are often developed on a separate track from the emissions inventories submitted to the EIS.
- Emissions thresholds, which exempt some facilities addressed in local-scale analyses from being reported to the NEI under the Air Emissions Reporting Rule (AERR).
- The perception that emissions inventory improvements made for local-scale analyses are of limited usefulness to agencies in other states.

These findings provide insight into reasons why the best-available emissions inventory information may not be reflected in EIS submittals and point to the need for additional investigation into the relationship between local-scale emissions inventories and the NEI and its uses.

#### 4. CONCLUSIONS

The SLRT agencies that participated in the local-scale emissions inventory focus group provided valuable, experience-based information on local-scale inventory development and fine-scale modeling issues. This information is useful for providing guidance to other SLRT agencies that will be undertaking local-scale analyses in the future, as well as for providing insight into the relationship between local-scale inventories and the NEI.

Regarding guidance for other SLRT agencies, the following actions were identified by focus group participants as a potential checklist for local-scale emissions inventory development:

- Start with what you know – begin by identifying emissions sources in your area of

interest using existing inventories, permit data, and other sources of information.

- Communicate with owners/operators of individual facilities early and often. Use multiple channels of communication, including letters and face-to-face meetings, to educate facility owners/operators on local air quality issues, the results of analyses that have evaluated their facility's impact on monitored pollutant concentrations, and the need for controls.
- Use simple approaches, such as emissions-to-distance (Q/D) analysis, to prioritize sources in terms of potential impact on monitoring sites.
- Understand your monitoring data thoroughly, particularly speciated data. Investigate the variation of species concentrations by site, season, hour, etc. before attempting more detailed analyses such as receptor modeling.
- When conducting analyses on local source contributions, use a weight-of-evidence approach combining the results of receptor modeling, wind analyses, and inter-monitor comparisons to zero in on sources with significant impacts on monitored concentrations.
- Take care to collect detailed information on stack parameters as well as emission rates. Work with facility operators to determine the best way to characterize sources for modeling, particularly fugitive sources.
- Perform a thorough quality assurance (QA) check on any data you receive from individual facilities. Talk to a permit engineer who understands the facility or industry to ensure that reported data are reasonable.
- Compare modeling results with results from other analyses (e.g., Q/D, PMF) to determine whether the modeling confirms earlier findings. If not, it may be necessary to re-evaluate modeled emissions rates or stack parameters.

Project findings also provided insight into the relationship between local-scale emissions inventories developed by SLRT agencies and the NEI. Focus group participants identified potential barriers that may prevent local-scale emissions data from reaching the EIS. These barriers

include timing issues, resource limitations, and the development of separate modeling inventories by agency modelers. As a result, the authors recommend further investigation into NEI data analyses that can support SLRT agencies developing more locally representative emissions data for fine-scale air quality modeling, as well as provide additional incentives to SLRT agencies to ensure that locally representative emissions data are reflected in EIS submittals.

## 5. REFERENCES

- Bacon L. and Cole L. (2010) *Alabama's local emissions inventory experiences. Presented to EPA's local-scale emissions inventory focus group, June 29.*
- Bohlmann B. and Rairigh K. (2010) *Ozone events in the Upper Green River Basin of Southwestern Wyoming. Presented to EPA's local-scale emissions inventory focus group, August 10.*
- Boylan J. (2010) *Local-scale PM<sub>2.5</sub> modeling in Atlanta. Presented to EPA's local-scale emissions inventory focus group, July 13.*
- Cook R., Isakov V., Touma J., Benjey W., Thurman J., Kinnee E., and Ensley D. (2008) *Resolving local-scale emissions for modeling air quality near roadways. J. Air & Waste Manage* **58**, 451-461.
- Georgia Department of Natural Resources (2010) *Georgia's proposed state implementation plan for the Atlanta PM<sub>2.5</sub> nonattainment area. Prepared by the Environmental Protection Division of the Georgia Department of Natural Resources, March.*
- Graham J. and Maranche J. (2010) *Local-scale emissions inventory focus group: ACHD responses to charge questions. Presented to EPA's local-scale emissions inventory focus group, July 13.*
- Maranche J. (2006) *Allegheny County PM<sub>2.5</sub> source apportionment results using the positive matrix factorization (PMF) model, version 1.1. Prepared by the Air Quality Program of the Allegheny County Health Department, January.*
- Norris G., Vedantham R., Wade K.S., Brown S.G., Prouty J.D., and Foley C. (2008) *EPA positive matrix factorization (PMF) 3.0 fundamentals and user guide. Prepared for the U.S. Environmental Protection Agency, Washington, D.C., by the National Exposure Research Laboratory, Research Triangle Park; Sonoma Technology, Inc., Petaluma, CA; and Lockheed Martin Systems Engineering Center, Arlington, VA, EP-D-05-004; STI-907045.05-3347-UG, October.*
- Reid S.B., Pollard E.K., and Du Y. (2010) *Emissions inventory development for the Cleveland Multiple Air Pollutant Study. Final report prepared for Alion Science and Technology, Durham, NC, by Sonoma Technology, Inc., Petaluma, CA, STI-910007-3909-FR, June 30.*
- Sprague J. (2010) *Granite City, IL, PM<sub>2.5</sub> nonattainment: regional and local-scale modeling, data analysis, and emissions control developments. Presented to EPA's local-scale emissions inventory focus group, July 27.*
- Tooly R.L. and Wesson K. (2009) *Local-scale emissions information for high resolution air quality modeling: Detroit multi-pollutant pilot project. Poster presented at the 18th Annual Emissions Inventory Conference, Baltimore, MD, April 14-27.*
- U.S. Environmental Protection Agency (2007) *Guidance on the use of models and other analyses for demonstrating attainment of air quality goals for ozone, PM<sub>2.5</sub>, and regional haze. Guidance document prepared by the U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC, EPA-454/B-07-002, April.*