FAIRMODE
Forum for air quality modelling in Europe

WG3-CCA: Source apportionment

Measurements & modelling

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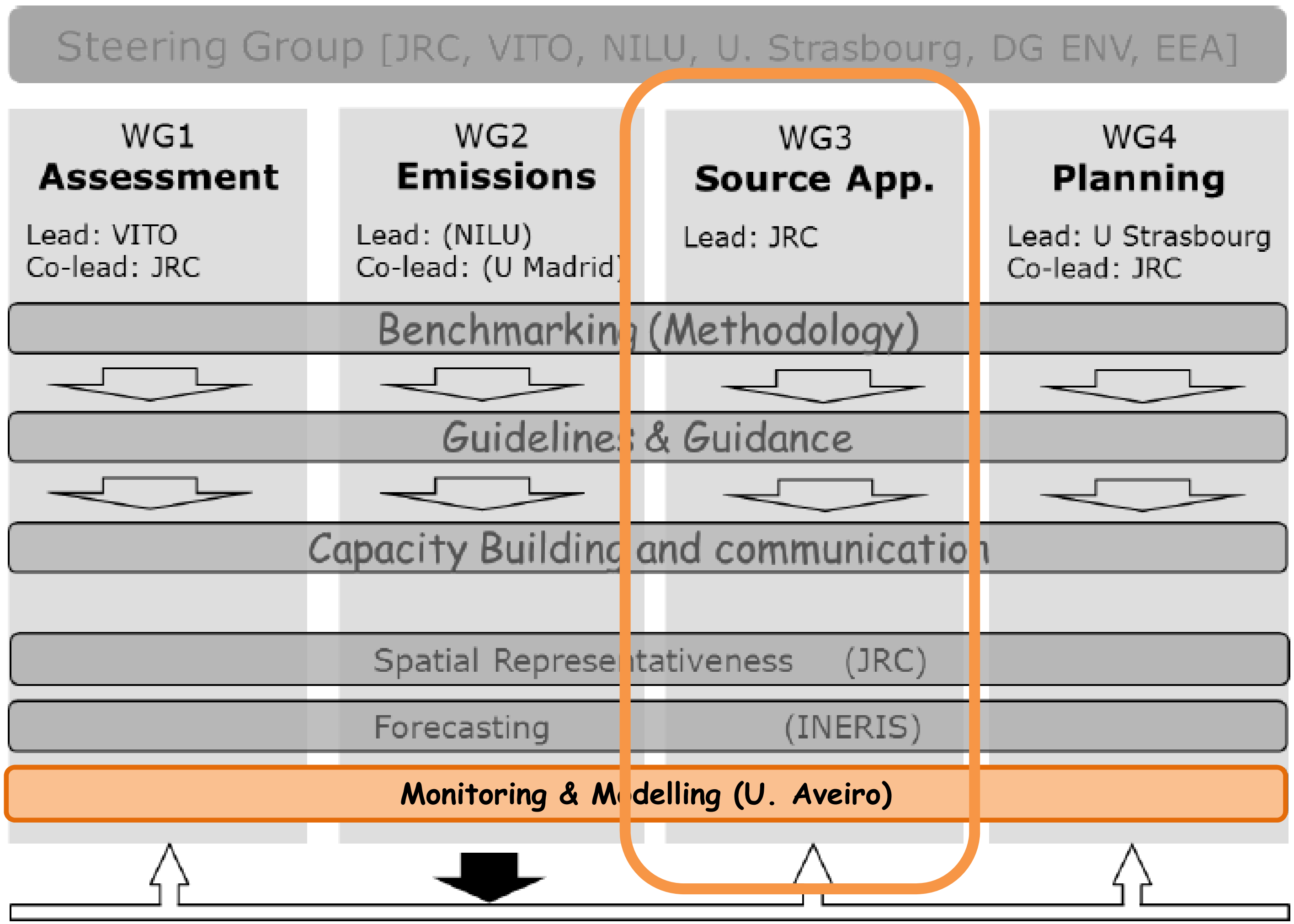
Objectives | FAIRMODE structure



Objectives | following last WG2-SG1…

To deal with inter-WG about the use of monitoring and modeling to support assessment and planning applications.

- To promote best practices on the combined use of models and monitoring for Directive related applications
- To develop and apply quality assurance practices when combining models and monitoring
- To provide guidance on station representativeness and station selection for the combined use of monitoring with modelling and for validation purposes
- …

Monitoring & Modelling: examples

Application 1: Assessment of air quality levels to establish the extent of exceedances and establish the population exposure

Application 2: Forecasting air quality levels for short term mitigation and public information and warnings

Application 3: Source allocation to determine the origin of AQ standard exceedances and provide a knowledge basis for planning strategies

Application 4: Assessment of plans and measures to control AQ exceedances

Data integration
(bringing together various data sources)

Data fusion
(statistical methods like bias correction)

Data assimilation
(monitoring data guide models)

Source:
Bruce and Spangl, 2010
WG2 FAIRMODE

Requests to participants | Meeting April 2014

1. REVIEWING METHODOLOGIES

- Update the compilation of monitoring & modelling practices/experiences

2. GUIDANCE ON MODEL VALIDATION WHEN USING M&M

- Common procedures to arrive at an independent model evaluation
- Quality control/quality assurance of the monitoring data

3. USE OF M&M FOR PLANNING PURPOSES

- List of planning exercises already applied and under study ("dynamic" evaluation)
- Experiences on using monitoring data for air quality management purposes

4. QUALITY OF MONITORING DATA: NETWORK QUALITY

- Criteria for the monitoring network
- Network design
- Problems and questions

In the meanwhile start thinking about emissions and SA

Q1. Can we use source apportionment methods to improve emission estimates?

Different approaches to source attribution of air pollutants:

(1) high-order emission-based source apportionment modeling

(2) an Area-of-Influence method for inverting concentration-emission relationships in chemical transport models (CTMs) to determine the sources impacting each receptor

(3) **a four-dimensional data assimilation (FDDA) method for using CTMs to improve emissions characterization:** refine and apply inverse modeling to improve emissions and source apportionment determinations

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Integrated Source/Receptor-Based Methods for Source Apportionment and Area of Influence Analysis

Research Project Search

NCER Research Project Search

EPA Grant Number: R832159
Title: Integrated Source/Receptor-Based Methods for Source Apportionment and Area of Influence Analysis
Investigators: Russell, Armistead G. , Odman, M. Talat
Institution: Georgia Institute of Technology
EPA Project Officer: Winner, Darrell
Project Period: December 27, 2004 through December 26, 2007
Project Amount: $444,899
RFA: Source Apportionment of Particulate Matter (2004)
Research Category: Air Quality and Air Toxics , Particulate Matter

Description:

Proposed is a study to capitalize upon recent advances in atmospheric modeling to develop and refine three innovative approaches to source attribution of particulate matter (PM): (1) high-order emission-based source apportionment modeling, (2) an Area-of-Influence method for inverting concentration-emission relationships in chemical transport models (CTMs) to determine the sources impacting each receptor, and (3) a four-dimensional data assimilation (FDDA) method for using CTMs to improve emissions characterization.

Objective:

Primary objectives of this research are to: 1) extend a recently developed, non-linear source apportionment method for ozone to $PM_{2.5/coarse}$ and apply it to various locations to provide long-term, daily source apportionments (SAs) across

Q2. How can we better profit from source oriented models?

Receptor-oriented statistical models are extensively used in air pollution source apportionment studies **based on concentrations measured at monitor locations**.

Provide an alternative bottom-to-top approach to quantify the contributions from different sources **based on existing emission inventories** and first-principle chemical transport models. The two approaches complement each **other to provide a more solid and complete understanding of air pollution problems** and their control strategies.

Q2. How can we better profit from source oriented models?

Example:
Source-oriented model in evaluating on-road vehicle emissions

Atmospheric Environment

Volume 85, March 2014, Pages 99–108

Evaluation of on-road vehicle CO and NO_x National Emission Inventories using an urban-scale source-oriented air quality model

Sri Harsha Kota[a], Hongliang Zhang[a, 1], Gang Chen[a], Gunnar W. Schade[b], Qi Ying[a]

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http://dx.doi.org/10.1016/j.atmosenv.2013.11.020

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Highlights

- On-road vehicle CO and NO_x inventories from MOBILE6.2 and MOVES were evaluated.
- Performance of CO and NO_x show clear tread as a function of vehicle contributions.
- CO and NO_x from MOBILE6.2 are over-estimated by 60% and 15–25%, respectively.
- The performance of the meteorology model affects emission inventory evaluation.

Abstract

The MOBILE6.2 model was replaced by the Motor Vehicle Emission Simulator (MOVES) in 2012 as an official tool recommended by the United States Environmental Protection Agency (US EPA) to predict vehicular pollutant emission factors. In this study, on-road vehicle emission inventories of CO and NO_x for Southeast Texas generated by MOVES and MOBILE6.2 in two versions of the 2005 National Emission

Q3. How to do the best use of monitored data to improve source apportionment (receptor and source oriented) results?

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Res Rep Health Eff Inst. 2010 Dec;(153):3-75; discussion 77-89.

Improved source apportionment and speciation of low-volume particulate matter samples.

Schauer JJ[1], Majestic BJ, Sheesley RJ, Shafer MM, Deminter JT, Mieritz M; HEI Health Review Committee.

Author information

Abstract

New chemical analysis methods for the characterization of atmospheric particulate matter (PM)* samples were developed and demonstrated in order to expand the number of such methods for use in future health studies involving PM. Three sets of methods were, developed, for the analysis (1) of organic tracer compounds in low-volume personal exposure samples (for source apportionment), (2) of trace metals and other trace elements in low-volume personal exposure samples, and (3) of the speciation of the oxidation states of water-soluble iron (Fe), manganese (Mn), and chromium (Cr) in PM samples. The development of the second set of methods built on previous work by the project team, which had in the past used similar methods in atmospheric source apportionment studies. The principal challenges in adapting these methods to the analysis of personal exposure samples were the improvement of detection limits (DLs) and control of the low-level contamination that can compromise personal exposure samples. A secondary goal of our development efforts was to reduce the cost and complexity of the three sets of methods in order to help facilitate their broader use in future health studies. The goals of the project were achieved, and the ability to integrate the methods into existing health studies was demonstrated by way of conducting two pilot studies. The first study involved analysis of trace elements in size-resolved PM samples that had been collected to represent study subjects' personal exposures along with simultaneous measures of indoor and outdoor PM concentrations. The second study involved analysis of the speciation of organic tracer compounds in personal exposure samples, indoor samples, and outdoor samples in order to understand the diesel PM exposure of study subjects in various job classifications in an occupational setting. Both pilot studies used existing samples from. large multi-year health studies and were intended to demonstrate the feasibility and value of using the new chemical analysis methods to better characterize the personal exposure samples. Analysis of the health data and the broader implications of the exposure assessments were not evaluated as part of the present study, but our pilot-study measurements are expected to contribute to investigators' future analyses in the large multi-year health studies. The methods we developed for the low-cost measurement of the oxidation states of Fe, Mn, and Cr in atmospheric PM samples are extremely sensitive and well suited for use in health studies. To demonstrate the utility of these methods, small-scale studies were conducted to characterize the redox cycling of Fe in PM on the time scale of atmospheric transport from source to personal exposure and to provide preliminary data on the atmospheric concentrations of soluble forms of the target metals in selected urban environments (in order to help focus future research seeking to understand the role of metals in human exposure to PM and its adverse health effects). The present report summarizes the methods that were developed and demonstrated to be suitable for use in health studies and provides pilot-scale data that can be used to develop hypotheses and experimental strategies to further enhance the ability of future health studies to elucidate the role of PM, PM sources, and PM components in the observed associations between atmospheric PM and adverse human health outcomes.

Q3. How to do the best use of monitored data to improve source apportionment (receptor and source oriented) results?

EXECUTIVE SUMMARY

This study analyzed air quality monitoring data from 16 sites in the northeastern quarter of the United States. The sites were chosen from among the IMPROVE (Interagency Monitoring of Protected Visual Environments) network and the CASTNET (Clean Air Status and Trends Network) sites operated by the U.S. EPA and Federal Land Managers in Federal Class I areas and rural areas. The basic objective of this study is to:

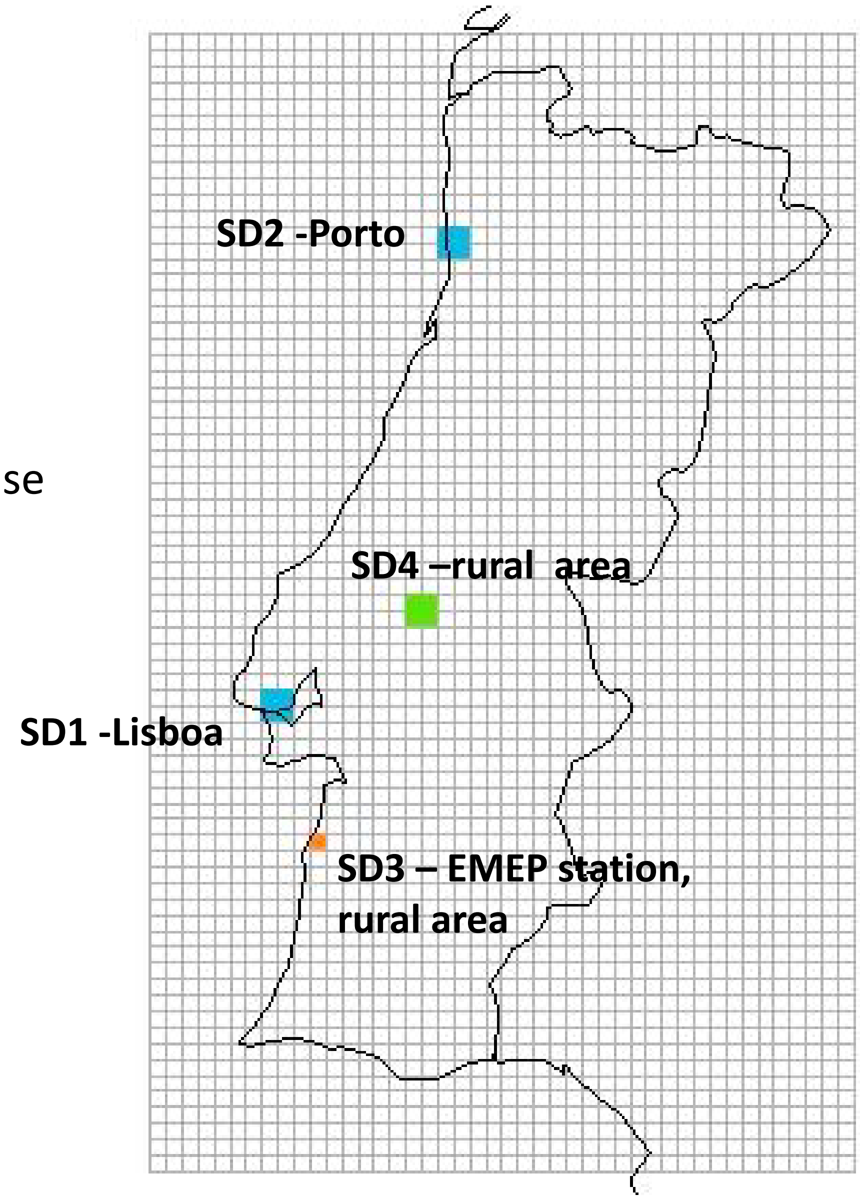
> Identify emissions sources and quantify their contributions to $PM_{2.5}$ and to light extinction during the 20 percent best and 20 percent worst visibility days in non-urban portions of the midwestern and eastern United States based on receptor observations.

Secondary goals to support the primary goal included: evaluating and screening available ambient measurements for modeling with receptor models, evaluating an existing emissions profile database for use in identifying the output from the models, and assessing the output from the models. The results are intended to help state and tribal authorities responsible for improving visibility at major national parks and wilderness areas. Collectively, this study, along with other air quality analyses, emissions inventory data, and emissions-based or meteorological modeling, should be considered in a "weight-of-evidence" assessment of the sources and contributions to fine particle and visibility impairment problems in the midwestern and eastern U.S.

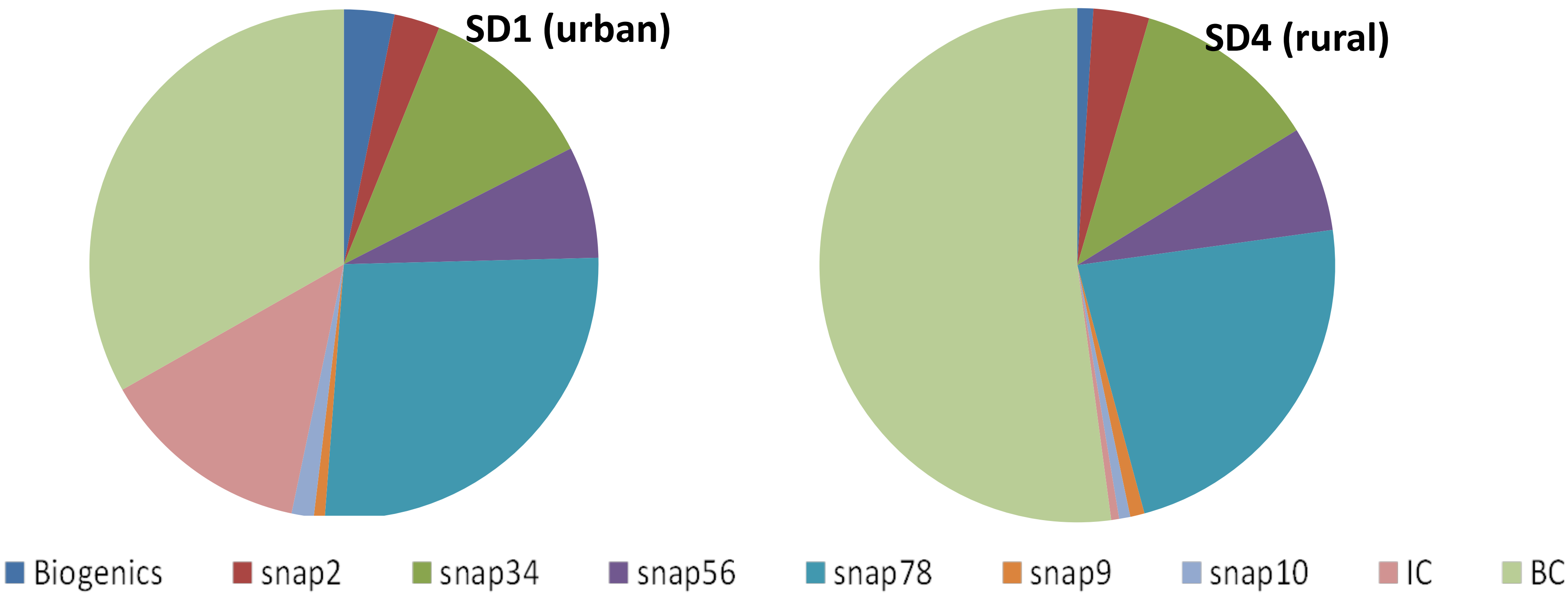
http://www.marama.org/visibility/SA_report/Sec1-3.pdf

Example of source apportionment exercise

- 4 receptor regions, corresponding to 4 SD
- 7 emission categories:
    - biogenic
    - non-industrial combustion (SNAP 2)
    - industry (SNAPs 3, 4)
    - distribution of fossil fuels and solvent use (SNAPs 5, 6)
    - transport (SNAPs 7, 8)
    - waste treatment and disposal (SNAP9)
    - agriculture (SNAP10)



Contribution of emissions, initial and boundary condition to ozone 8h daily maximum concentration



- source contribution is different between subdomains
- traffic (SNAPS 7 and 8) more important in the urban area
- BC more important in the rural area