Lesson X. Introduction To The CMB8 Software.

Peter Scheff
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Goal

To become familiar with the CMB8 software and the commands necessary to run the model.

Lesson Objectives

- Learn how to install CMB8 software onto a PC.
- Describe the necessary input files for the CMB program.

Lesson Objectives

- Describe the structure of the input and output files for the CMB8 computer program.
- Explain the functions of the CMB8 commands.

CMB8 Overview

- Development sponsored by USEPA Office of Research and Development and Office of Air Quality Planning and Standards.
- Developed by Desert Research Institute.
- Began development in 1996.

CMB8 Overview

- Approved as a regulatory planning tool for the development of State Implementation Plans.
- Since 1990, EPA has distributed CMB7 freely on SCRAM regulatory models clearinghouse.

CMB8 Overview

Ftp://ttnftp.rtpnc.epa.gov/e-drive
/scram/cmb7/cmb7.zip
cmb7d.zip
readme.txt

CMB8 Overview

- New code currently available via anonymous ftp:
- ftp://eafs.sage.dri.edu/currproj/CMB80 /model/CMB832.exe

CMB8 Overview

- ftp://eafs.sage.dri.edu/currproj/CMB80 /model/CMB816.exe

Improvements Over Previous Versions

- Windows Based
  - Either 3.x (16 bit) or Windows 95' (32 bit) Code.
  - Will not be available for DOS environment.

Improvements Over Previous Versions

- User friendly interface.
- Designed for particulate matter and VOC applications.

Improvements Over Previous Versions

- Increased formatting options for the large input files.

(including .TXT, .CAR, .CSV, .DBF, and .WKS or .WK1)

Improvements Over Previous Versions

- New options for output files. (files can be renamed and directed to different directories)
- Up to ten sets of source and species selection defaults can be specified.

Improvements Over Previous Versions

- Increased flexibility in handling collinearity problems. (defaults are no longer hard-wired)
- Britt-Leuke Algorithm without approximation is now available.

Improvements Over Previous Versions

- Restart option allows uncompleted session to be resumed.
- Improvements in graphical display.
- Automatic source elimination option. (to remove negative source contributions)

Improvements Over Previous Versions

- Measurement units and number of decimal places can now be specified.

Installation of CMB For Windows 3.x

- Enter file manager in windows.
- Click on C drive. (or alternate hard drive choice)
- Create directory in hard drive. (c:\CMB8)

Installation of CMB For Windows 3.x

- Click on drive or directory which contains the CMB8 software.
- Drag CMB8 software file to the CMB8 hard drive directory.

Installation of CMB For Windows 3.x

- Run the CMB816.exe file to create files.
- To run the program, click on CMB8.exe file or create an icon and Program Group for CMB8 program. The program can be started by double clicking on the icon.

Installation of CMB8 For Windows 95'

- Within Windows Explorer, highlight drive/directory where program will be installed, select File Menu, New Folder and create CMB8 folder.
- Copy CMB8 software to CMB8 directory.

Installation of CMB8 For Windows 95'

- Double click on CMB832.exe to create program files.
- To run program:
  - Double click on CMB8.exe in CMB8 directory .

    OR
  - Add program to start menu.

Installation of CMB8 For Windows 95'

- To add program to start menu:
  - press start button
  - select settings
  - select taskbar
  - select start menu programs
  - push add

Installation of CMB8 For Windows 95'

- To add program to start menu:

  insert complete path to CMB8.exe
  place in Programs (or other) folder

Installation of CMB8 For Windows 95'

- The other option is to create a short-cut.
- To create a short-cut on desk top:
  - open windows explorer
  - highlight CMB8.exe in CMB8 directory

Installation of CMB8 For Windows 95'

- To create a short-cut on desk top:
  select create shortcut in file menu
  drag shortcut to CMB8 onto the desk top

Input Files

Six files are necessary:

- .in8 file to identify input files
- Ambient data file
(.txt, .car, .csu, .dbf, .wks, or .wk1)

Input Files

- Source profile data file
(same options as ambient data)
- Species selection file (.sel)
- Source selection file (.sel)

Input Files

- Ambient sample selection file (.sel)
- INPUT FILE
  INXXXXXX.IN8

  where: XXXXXX = name

Input File

- INXXXXXX.IN8 contains the names of files
  SOXXXXXX.SEL
  POXXXXXX.SEL
  ADXXXXXX.SEL
  ADXXXXXX.TXT
  PRXXXXXX.TXT

Selection Files

- SOURCE PROFILE SELECTION FILE
  SOXXXXXX.SEL

Field:

1	6-character source code number	1-6
2	8-character profile name	9-16
3	include in initial model	19
4	comments	21-80

Selection Files

- SPECIES SELECTION FILE
  POXXXXXX.SEL

Field 1:	6-character species code	1-6
Field 2:	8-character species name	9-16
Field 3:	include in initial model	19
Field 4:	comments	21-80

Selection Files

- AMBIENT DATA SELECTION FILE
  ADXXXXXX.SEL

Field 1:	Site ID, up to 12 characters	
Field 2:	Sampling Date	AA/BB/CC
Field 3:	Sample Duration	YY
Field 4:	Sample start hour	ZZ

Selection Files

Filed 5: Size Fraction VVVVV

Field 6: columns 37-46
east/west coordinates

Field 7: columns 48-57
north/south coordinates

Selection Files

- Coordinates are optional
- Use floating point format
- Increase in value from left to right and from top to bottom
- UTM coordinates are suitable

Ambient Data File

- ADXXXXXX.YYY

where: XXXXXXX = name
YYY = file type

Ambient Data File

- Valid file types
  - .txt blank delimited text
  - .car column and row reversed text
  - .csv column separated value text
  - .dbf data base file
  - .wks lotus spreadsheet

Ambient Data File

Field 1: Site ID, 12 characters max

Field 2: Sample date, 8 characters max

Field 3: Sample duration, 2 characters max

Field 4: Sample start hour, 2 characters max

Ambient Data File

Field 5: Size fraction, 5 characters max
(up to 4 different are allowed)

Field 6: Mass concentration

Field 7: Precision of mass concentration

Ambient Data File

Field 8+2n: concentration of species *i*,
from *I* =1 to n
(missing value = -99)

Field 9+2n: precious of species *i*,
from *I* = 1 to n
(must be greater than zero)

Source Profile Data File

- PRXXXXXX.YYY

where: XXXXXXX = name
YYY = file type
(.txt, .car, .csv, .dbf, or .wks)

Source Profile Data File

Field 1: Profile number or source code, 6 characters max

Filed 2: Source name, 8 characters max

Field 3: Size (PM10, RP,CP,TVOC,....), 5 character max

Source Profile Data File

Field 4+2n: Fraction of species n in primary mass of source emission

Field 5+2n: Variability of species in primary emission (must be greater than zero)

Source Profile Data File

- Recommended default:
  0 for mass fraction
  0.0001 for variability

Functions of CMB8

- Upon initial start-up, CMB prompts for restart from previous session.
- Selection of a specific file.
- Click yes and select input file.

Functions of CMB8

- CMB8 menu window appears.

Functions of CMB8
'SAM'

- First step in running software.
- Allows for selection of ambient data records for analysis.
- Selection indicated by *.

Functions of CMB8
'SAM'

- Must select sample before progressing further.
- Top selected ambient data record will be fit first.

Functions of CMB8
'SAM'

- Current selected sample is displayed on line below Function buttons.

Functions of CMB8
'ADV'

- Advances to the next available sample.
- Current sample selected display is updated.

Functions of CMB8
'SPE'

- Allows for selection of fitting species.
- Selection indicated by *.
- Default selection specified in species selection file are initially selected.

Functions of CMB8
'SPE'

- Species can be added or removed.
- Can change selection using the 'Modify' button.

Functions of CMB8
'SRC'

- Allows for selection of sources.
- Selection indicated by *.
- 'Defaults' button brings up the 10 default selections of the fitting species.

Functions of CMB8
'SRC'

- Sources can be added or removed.
- Can change selections using the 'Modify' button.

Functions of CMB8
SAM, SPE, SRC Similarities

- Can select all or deselect all.
- Each menu must be deactivated by clicking OK before progressing further.

Functions of CMB8
'FIT'

- Performs CMB calculation on selected sample using sources and species selected.
- Displays
  - Source contribution estimated
  - Regression diagnostics (R square, chi square, % mass)

Functions of CMB8
'FIT'

- Displays
  - Collinearity diagnostics
  - Measured and calculated species concentrations
  - Ratio calculated and measured

Functions of CMB8
'FIT'

- Writes results in windows buffer.
- Must write, print, and clear before buffer fills.

Functions of CMB8
'AUT'

- Autofit
- Solves CMB sequentially for each sample selected.

Functions of CMB8
'AUT'

- Automatically writes to:

CMBOUTRP.TXT
CMBOUTDB.TXT

Functions of CMB8
'SCN'

- Displays source contributions for last CMB calculation.
- Displays for each source.
- Writes matrix to windows buffer.

Functions of CMB8
'AVG'

- Computes average of CMB calculations for session.
- Writes to windows buffer.

Functions of CMB8
'PRO' and 'RCN'

- PRO -
  Writes source profile matrix to buffer.
- RCN -
  Writes current measured concentrations to buffer.

Functions of CMB8
'MPN'

- Writes transpose of sensitivity matrix to buffer.

Output Files

CMBOUTRP.TXT

- Text file
- Organized by sample

Output Files

CMBOUTRP.TXT

- Contains
  - Source estimates
  - Collinearity information
  - measured/calculated values by species

Output Files

CMBOUTDB.TXT

- Text file
- Organized by species

Output Files

CMBOUTDB.TXT

- Contains
  - ID
  - total concentration
  - contribution by source

Output Control Buttons

Clear	Clears window buffer
Clear Last	Clears last entry in buffer
Write RP	Writes to CMBOUTRP.TXT

Output Control Buttons

Write Last	Writes last entry to CMBOUTRP.TXT
Write DB	Writes to CMBOUTDB.TXT

Output Control Buttons

Print	Prints window buffer to default printer (Default font courier 10 point)
Print Last	Prints last entry
Close	Closes output window

Options

- Iteration Delta = 20
  Specifies max number of iterations
- Display Dec's (<=6)
  Sets number of decimals in output

Options

- Max Source Unc (%)
  Range 0-100% default = 20
- Min Source Proj
  Range 0-1 default = 0.95

Options

- RP Name
  Specifies name of CMBOUTRP.TXT
- DB Name
  Specifies name of CMBOUTDB.TXT

Options

- Units Specifies units
- B and L
  Selection causes CMB8 to use Britt and Luecke algorithm

Options

- S Elim
  Eliminates sources with negative coefficients
- Best Fit
  Automatically finds "best fit" - selects solution with largest fit measure

Options

- Weights
  Weights for best fit selection
- Output Format
  .TXT, .CSV, .DBF or .WKS

Options

- Output Directory
  Directory into which output is written

Graph Menu

Species

- Shows species concentrations for measured receptor concentrations
- Uses log-scale

Graph Menu

Source Profiles

- Shows source profile for a selected source

Graph Menu

Source Contributions

- Pie chart of current fit
- Sum of concentrations for selected sources are normalized to 100%

Graph Menu

PM10

- Produces a pie-chart for size total if the last two sizes were FINE and COARS.

Graph Menu

Time Series

- Graphs results from autofit
- Presented as stacked bar charts

Graph Menu

Spacial Pies

- Graphs a series of CMB solutions by location of receptor sites

Graph Menu

Graph Window

Allows the following commands:

- Print - sends current item to printer

Graph Menu

- Clip - copies current graph to the clipboard

- Orient - toggles between landscape and portrait

Lesson XI

Demonstration of the CMB Model Using CMB 8 Software

Peter Scheff

INTRODUCTION TO RECEPTOR MODELING

Lesson Title: Demonstration of the CMB model using CMB8 software
Lesson: XI
Prepared By: P.A. Scheff
Date: February 12, 1998

Lesson Goal: The goal of this lesson is to solve the chemical mass balance model and generate an output report using the CMB 8 software.

Lesson Objectives: At the completion of this lesson students will be able to:

Format input data files.

Use the appropriate commands to select ambient data, fit species, and obtain source fingerprints.

Solve the mass-balance equation using the CMB8 program.

Generate a report using the CMB8 program.

Regression diagnostics to evaluate model output.

Equipment Needs: A PC with modem for Internet connection.

Lesson XII

Receptor Model Evaluation and Validation
Richard Wadden

INTRODUCTION TO RECEPTOR MODELING

Lesson Title: Receptor Model Evaluation and Validation
Lesson: XII
Prepared By: R. Wadden
Date: February 12, 1998

Lesson Goal: CMB modeling results need to be validated to be sure the model reflects what is actually occurring in the environment. This session describes and demonstrates the various methods which may be used to compare CMB results with independently determined observations which reflect the same emission and meteorological phenomena.

Lesson Objectives: At the completion of this lesson students will be able to:

Explain the necessity for validating CMB receptor modeling results.

Explain why it is important to understand the emission source location and wind direction patterns within the airshed being evaluated by CMB modeling.

Compare results from diffusion modeling and receptor modeling based on the EPA SIP guidelines.

Use at least 3 techniques for comparing emission inventories and emission rates for specific source categories with receptor model results.

Lesson XII. Receptor Model Evaluation and Validation

Richard Wadden
University of Illinois at Chicago

1. Need for Validation

- Want to be sure model reflects what is actually occurring.

a. If receptor is downwind of a major source, e.g. a refinery, the CMB allocation should indicate significant refinery contributions.

1. Need for Validation

b. By the same token, if a receptor is upwind of a source, the contributions from that source category should be reduced.

C. The receptor model results need to be consistent with source-based modeling.

1. Need for Validation

- Resolving apparent differences ordinarily will provide more insight into air shed emissions.

2. Types of Validation

Want to compare with observations which are independent of ambient measurements and CMB modeling.

For example, emission inventories require a specific methodology and set of observations different from ambient measurements and CMB protocol.

2. Types of Validation

Agreement between the two strengthens our confidence in both; resolving differences provides us with a better understanding of the dynamics of a particular air shed.

2. Types of Validation

a. Point Sources - wind direction/wind speed trajectory analysis from known sources, e.g. power plants.

2. Types of Validation.

b. Emission inventory - if enough samples are gathered at one or more locations, the likelihood that a representative distribution of wind direction has been sampled. Under these conditions, the average values of the source coefficients provide an estimate of the emission inventory.
(For any given sample, however, the resulting source allocation will be very much dependent on the wind direction).

2. Types of Validation

c. Comparison with other parameters which should be related- For example, we would expect dust particulate levels to be higher with higher windspeeds.

Point Source Trajectory Analysis

- Chicago incinerators
- Tokyo oil refineries
- Chicago oil refineries
- Detroit coke ovens
- Chicago printing plants

Point Source Trajectory Analysis

- Chernivtsi, Ukraine, sulfur oxides
- Chernivtsi, Ukraine, welding aerosol
- Chernivtsi, Ukraine, graphite dust

Comparison with Emissions Inventories

- VOC Emission Inventories and Source Coefficients for:
  - Detroit - 1988
  - Chicago - 1986-1987
  - Beaumont - 1984-1987
  - Detroit - 1993
  - Chicago - 1991

Comparison With Other Parameters

- Windspeed and total or inhalable particulate
- Ambient silicon concentrations and soil allocation of PM_{10}
- Diesel particle allocation and weekend/weekday pattern

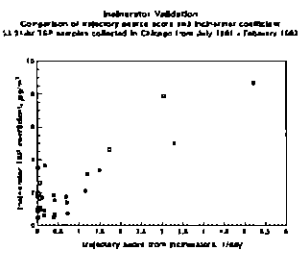
Comparison With Other Parameters

- For simultaneous NMOG and PM_{10} samples, comparison of the allocation of organics and allocation of PM_{10} for vehicles.

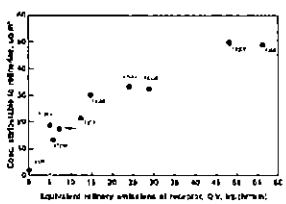
2.a. Point Source Trajectory Analysis

- Chicago incinerators
- Tokyo oil refineries
- Chicago oil refineries
- Detroit coke ovens
- Chicago printing plants

Point Source Trajectory Analysis
Scheff et al, Environ.Sci.Technol.,18,923, 1984



Point Source Trajectory Analysis
Wadden et al, Environ.Sci.Technol.,20,473-483, 1986

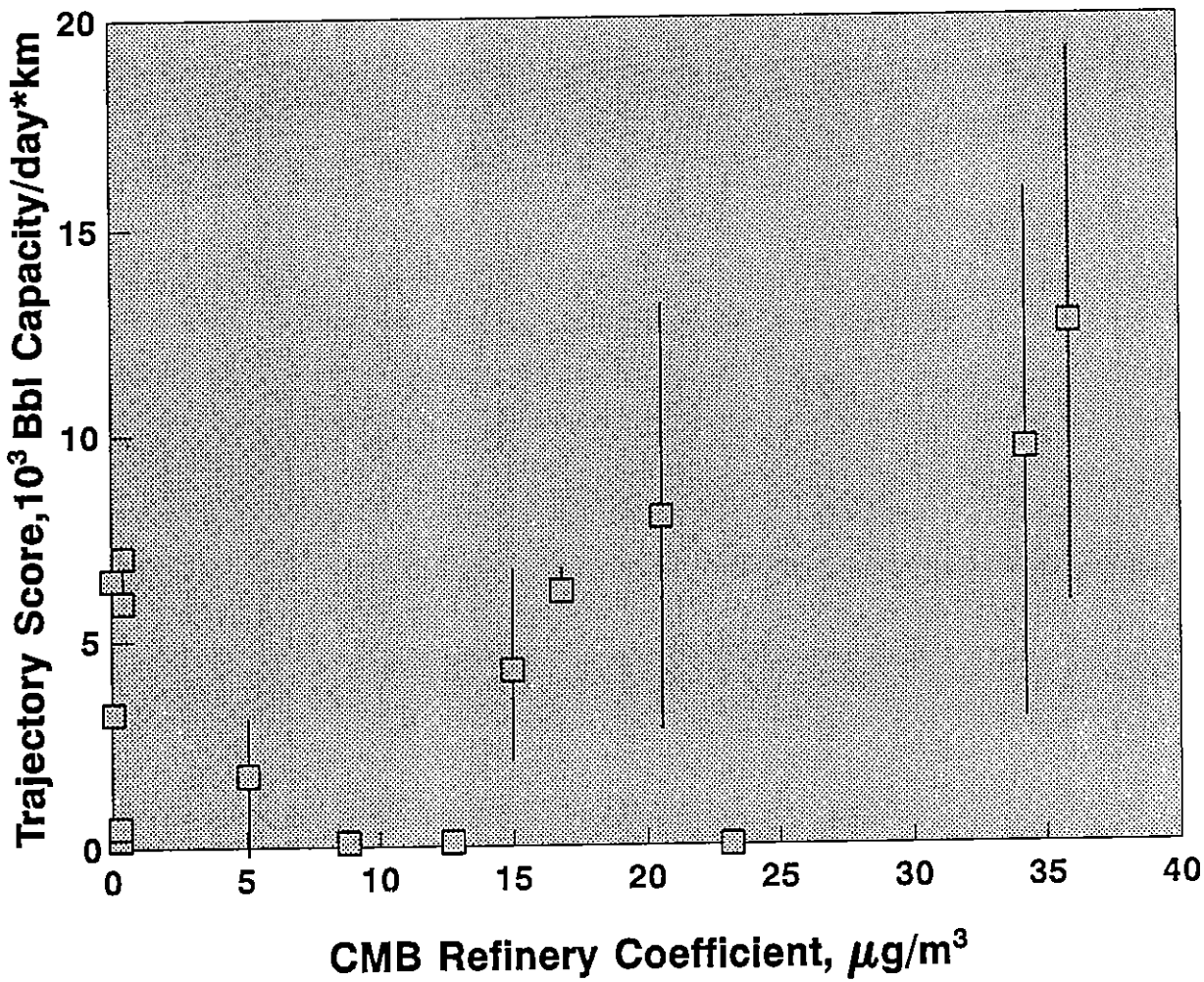


2.a. Point Source Trajectory Analysis

See Insert: Chicago, 1987: Relationship between trajectory score based on capacity and CMB coefficient for summer-time refinery emissions.

Point source trajectory analysis

Scheff and Wadden, Environ.Sci.Technol.,27,617, 1993



Chicago, 1987: Relationship between trajectory score based on capacity and CMB coefficient for summer-time refinery emissions at the central (SPH) receptor site.

2.a. Point Source Trajectory Analysis

See Insert: Detroit, 1988: Average Daily Coke Coefficients vs. Average Daily Trajectory Scores

2.a. Point Source Trajectory Analysis

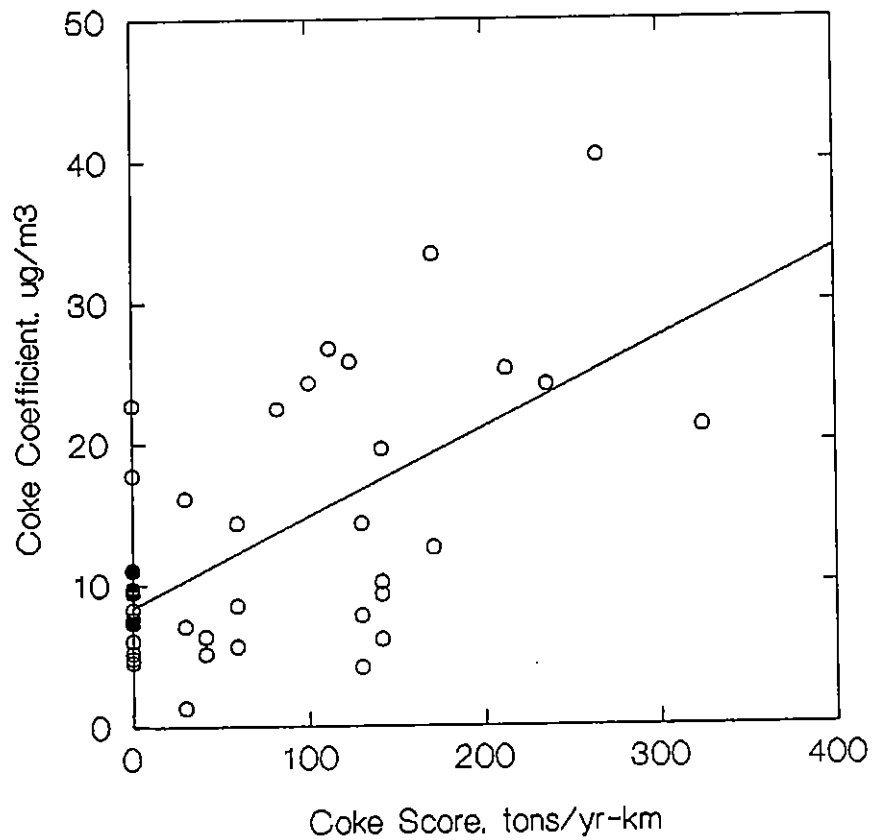
See Insert: Chicago, 1987: Relationship between trajectory score based on capacity and CMB coefficient for summer-time graphic arts emissions.

2.a. Point Source Trajectory Analysis

- Chernivtsi, Ukraine, sulfur oxides
- Chernivtsi, Ukraine, welding aerosol
- Chernivtsi, Ukraine, graphite dust

Point source trajectory analysis

Kenski et al, J.Environ.Engin.,121,483,1995



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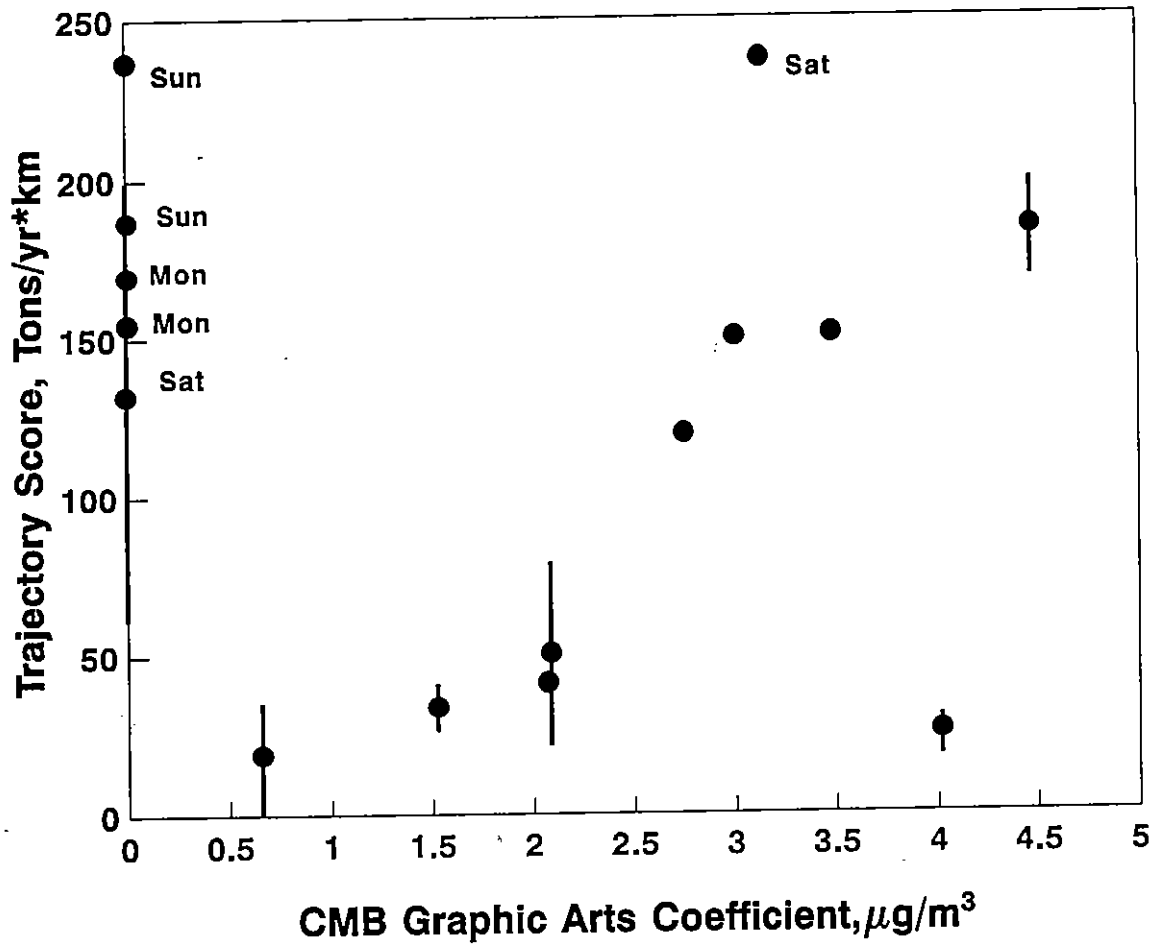
Point source trajectory analysis

Scheff and Wadden, Environ.Sci.Technol.,27,617, 1993



Chicago, 1987: Relationship between trajectory score and CMB coefficient for summer-time graphic arts emissions at the central (SPH) receptor site.

2.a. Point Source Trajectory Analysis

See Insert: 30 industrial plants with sulfur emissions

2.a. Point Source Trajectory Analysis

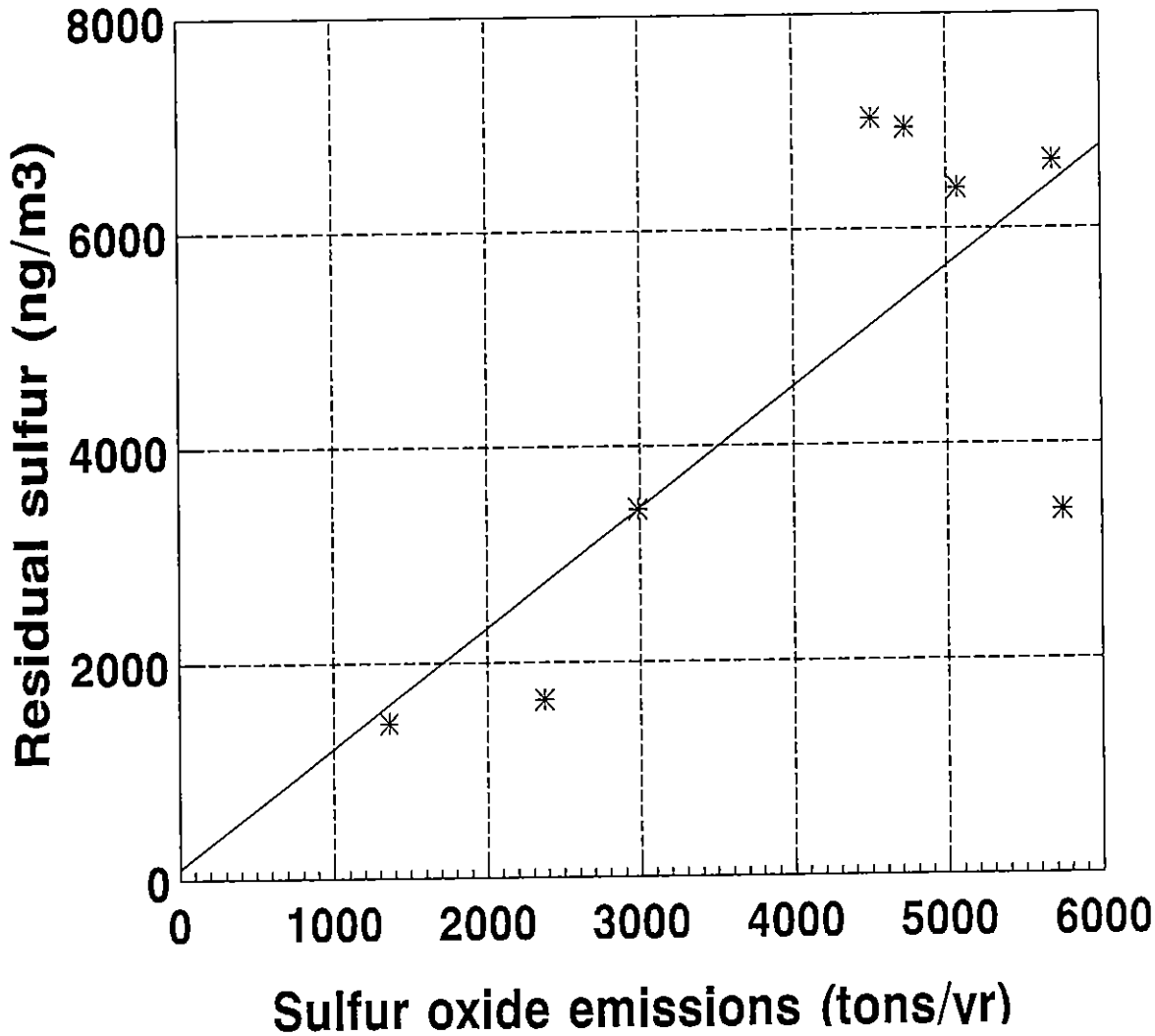
See Insert: 33 factories with welding emissions

2.a. Point Source Trajectory Analysis

See Insert: Factory emission of graphite dust

Chernivsti, Ukraine

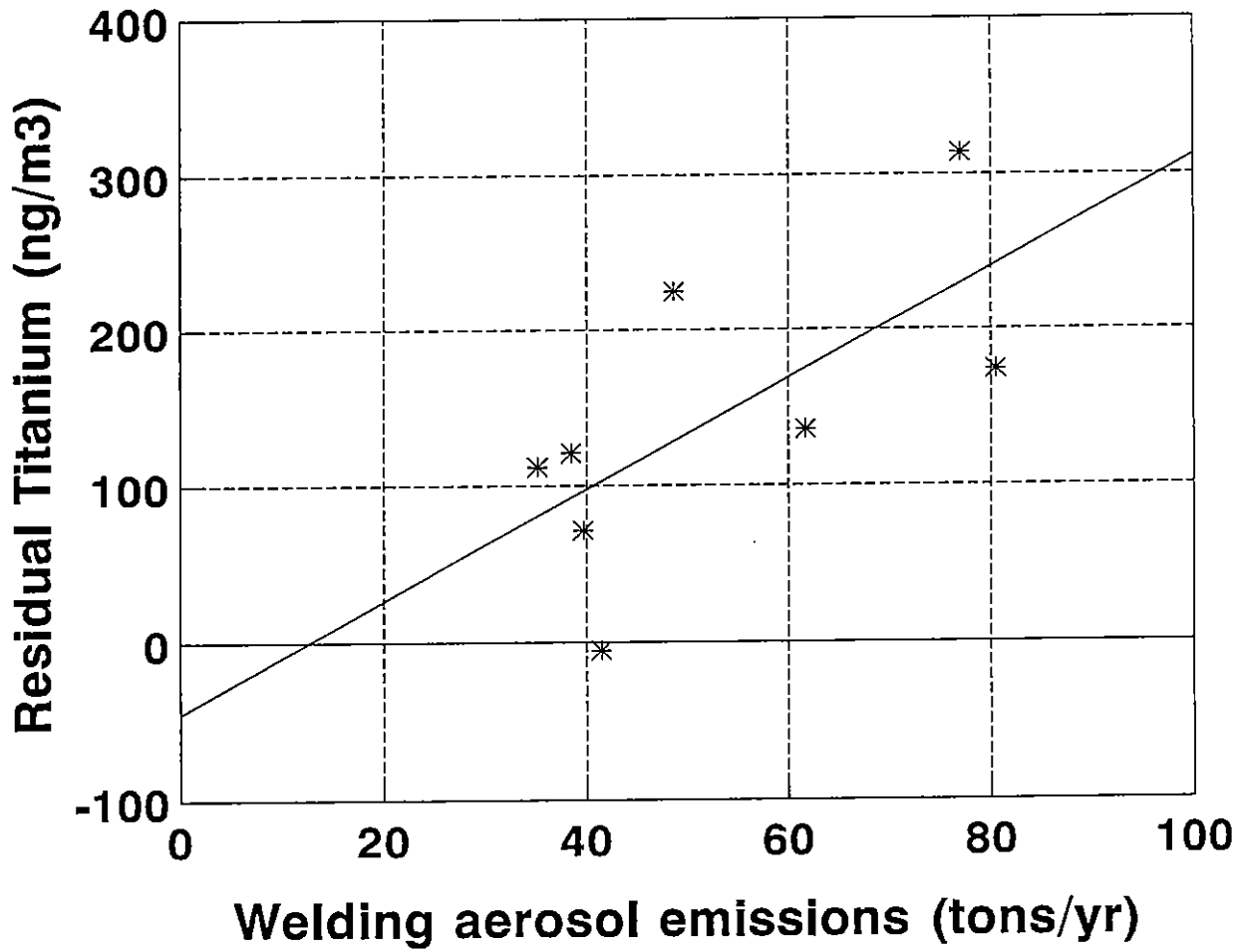
Scheff et al, Environ.Internat.,23,273-290, 1997



30 industrial plants with sulfur emissions.

Chernivsti, Ukraine

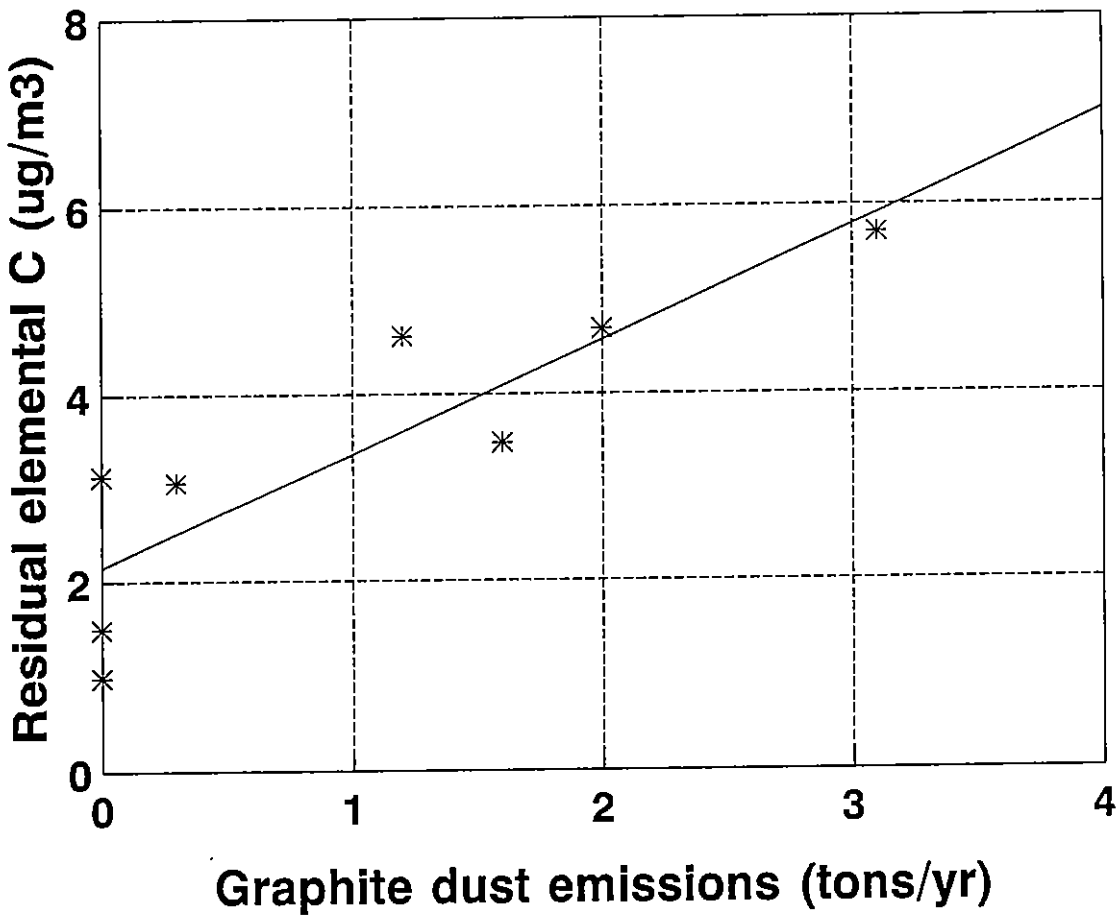
Scheff et al, Environ.Internat.,23,273-290, 1997



33 factories with welding emissions.

Chernivsti, Ukraine

Scheff et al, Environ.Internat.,23,273-290, 1997



Factory emissions of graphite dust.

2.b. Comparison with Emissions Inventories

- VOC Emission Inventories Average Source Coefficients for:

  Detroit- 1988
  Chicago - 1086-1987
  Beaumont - 1084-1987
  Detroit - 1993
  Chicago - 1991

2.b. Comparison with Emissions Inventories

Receptor Modeling approach to VOC Emission Inventory Validation - Kenski et al, J. Environ. Engin., 121, 483-491, 1995

2.b. Comparison with Emissions Inventories

See Insert Table For Detroit, Chicago, and Beaumont

2. Validation - CMB results compared with Inventory

	Detroit		Chicago			Beaumont	
Source	Emiss.[A] Inventory	Avg. Coef. (n=192)	Emission Inventory	Avg. Coef. (n=64)	Previous Study Coef. (n=55)	Emiss.[B] Inventory	Avg. Coef. (n=61)
Vehicles	32.9	28.2	35.1	41.2	33.8	11.9	13.6
Gasoline Vapor	6.9	9.4	7.6	11.7	6.4	4.2[b]	19.5
Oil Refinery	0.7	16.5	1.3	13.5	7.6	23.1	9.1
Arch. Coatings	3.8	2.5	5.5	6.2	3.1	-	0.6
Graphic Arts	0.7	4.7	9.8	11.0	6.6	-	1.4
Polyethylene	-	-	-	-	-	7.3	7.0
Coke Ovens	2.0	3.7	-	-	-	-	-
Other	53.0	34.5	40.6	16.5	-	53.5	48.8

[A]Canadian refinery emissions not included. Industrial coatings operations (14% of total) are not included in arch. coatings inventory estimate. [B]Gasoline vapor estimate is for point sources only.

2.b. Comparison with Emissions Inventories

Scheff et al, Receptor Model Evaluation of the Southeast Michigan Ozone Study Ambient NMOC Measurements,
J. Air & Waste Manage. Assoc., 46, 1048-1057, 1996.

2.b. Comparison with Emissions Inventories

See Insert : 1993 SEMOS Inventory and Average CMB Solution for Wayne County Monitors, wt%

2.b. Comparison with Emissions Inventories

[A]1993 SEMOS modeling emission inventory for the grid cells containing the Linwood (Wayne 04), Temple (Wayne 62) and E7 (Wayne 01) grid cells, and the surrounding grid cells.

[B]Average CMB solution for all SEMOS measurements at the three Wayne County sites.

[C]The Mararthon refinery, which is located in Wayne Co, is outside of the grid cells surrounding the SEMOS monitors.

2. Validation - CMB results compared with Inventory

1993 SEMOS Inventory and Average CMB Solution for Wayne County Monitors, wt %.

	1993 Emission Inventory for the Wayne County Monitor Locations[A]		CMB: Wayne County Monitors Average[B]	
Source Categories	Inventory Categories	Combined Vehicles + Gasoline	CMB Categories	Combined Vehicles + Gasoline
On-road/Off-road Vehicles	37.7		38.4	
Liquid Gasoline (vaporized)		46.3	6.1	46.3
Gasoline Vapor	9.06		1.8	
Refineries	0[C]		7.0	
Graphic Arts	0.64		4.1	
Architectural Coating	6.34		4.9	
Coke Ovens	1.88		2.9	
Other Sources	44.3		33.3	

2.b. Comparison with Emissions Inventories

Kenski et al, Using Ambient Data to Examine Emission Inventories: A Mass Balance Approach, AWMA Paper 96 FA149.01, Nashville, 1996.

2.b. Comparison with Emissions Inventories

See Insert : Figure 36

2.b. Comparison with Emissions Inventories

See Insert : Figure 37

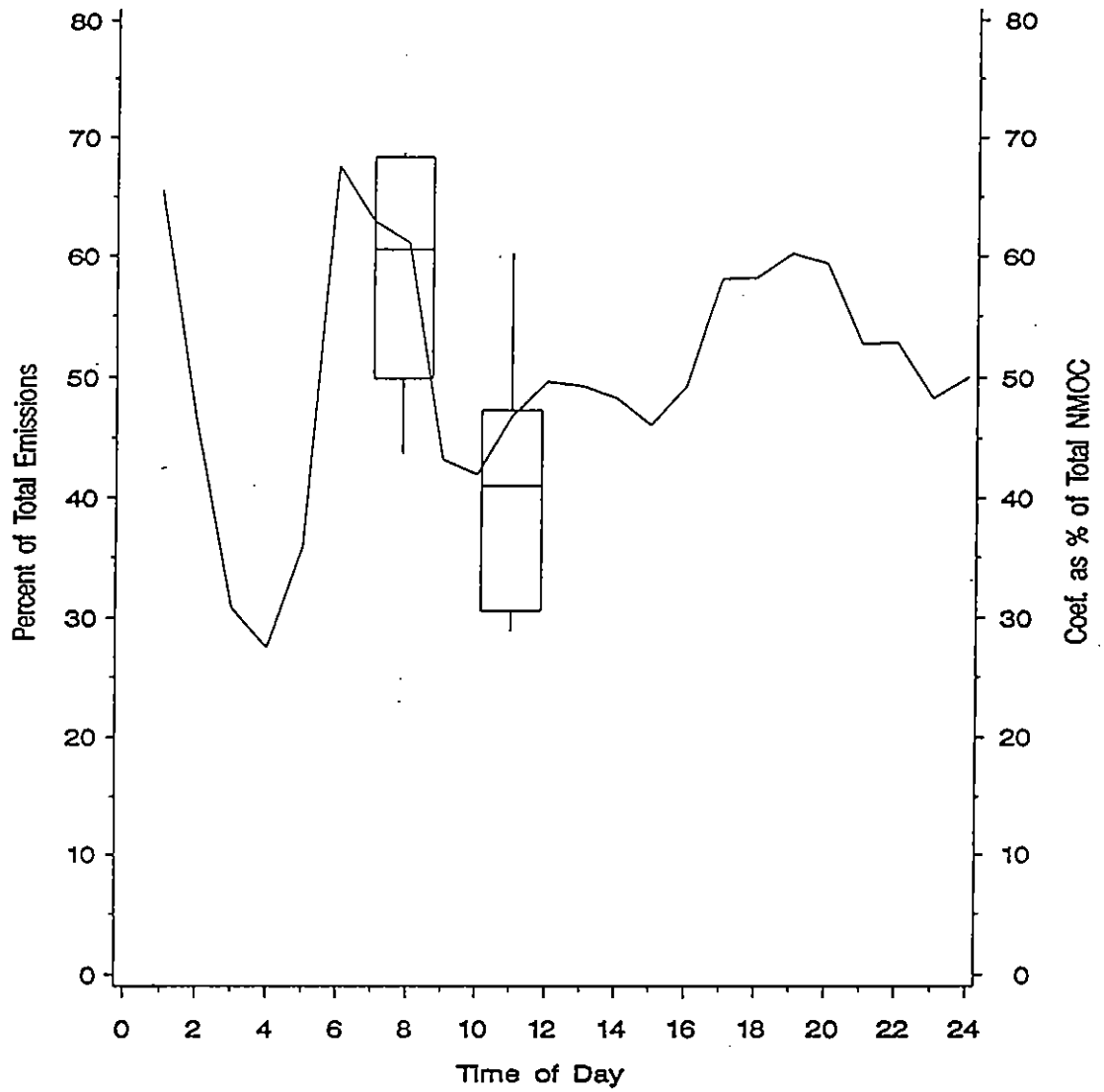


Figure 36. Comparison of LMOS Emission Inventory (solid line) and Receptor Model Emission Inventory (box plots) for Chicago Vehicles

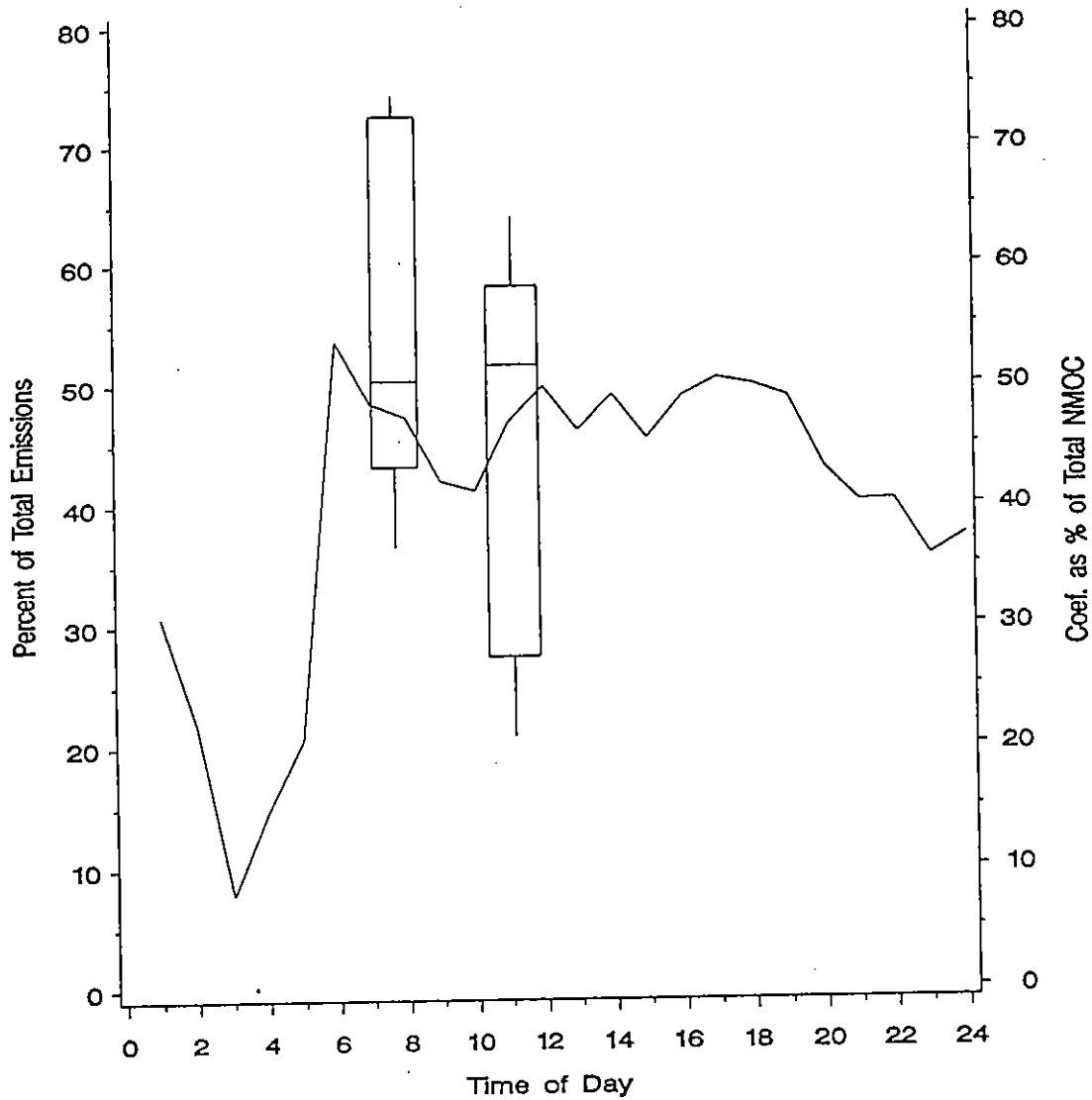


Figure 37. Comparison of LMOS Emission Inventory (solid line) and Receptor Model Emission Inventory (box plots) for Gary Vehicles

2.b. Comparison with Emissions Inventories

See Insert : Figure 38

2.c. Comparison With Other Parameters

- **Windspeed and total or inhalable particulate**
- **Ambient silicon concentrations and soil allocation of PM_{10}**
- **Diesel particle allocation and weekend/weekday**

2.c. Comparison With Other Parameters

- **For simultaneous NMOG and PM_{10} samples, comparison of the allocation of organics and allocation of PM_{10} for vehicles.**

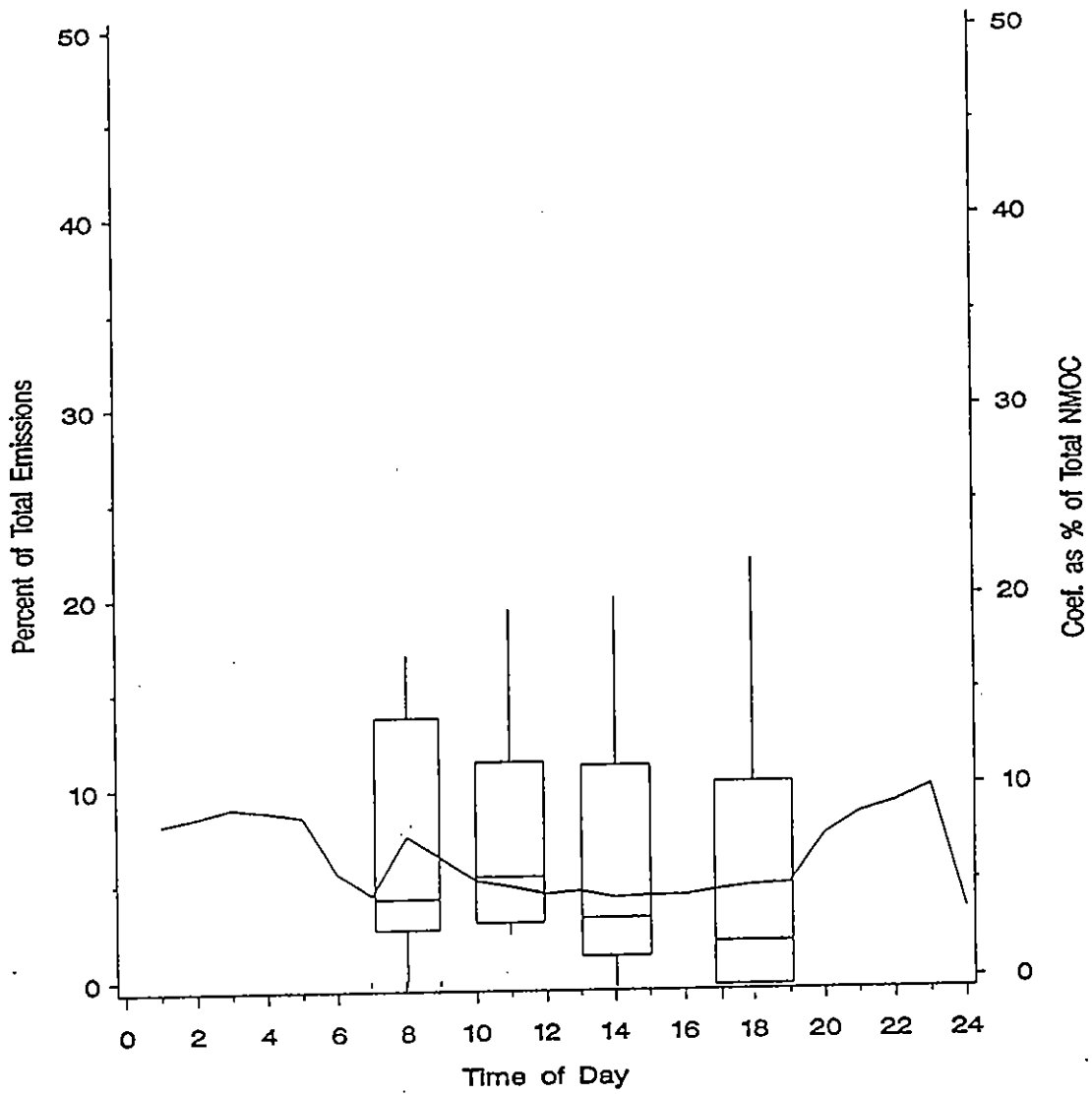


Figure 38. Comparison of LMOS Emission Inventory (solid line) and Receptor Model Emission Inventory (box plots) for Borculo Gasoline Storage and Transport

2.c. Comparison With Other Parameters

See Insert: Windspeed and Soil Coefficient

2.c. Comparison With Other Parameters

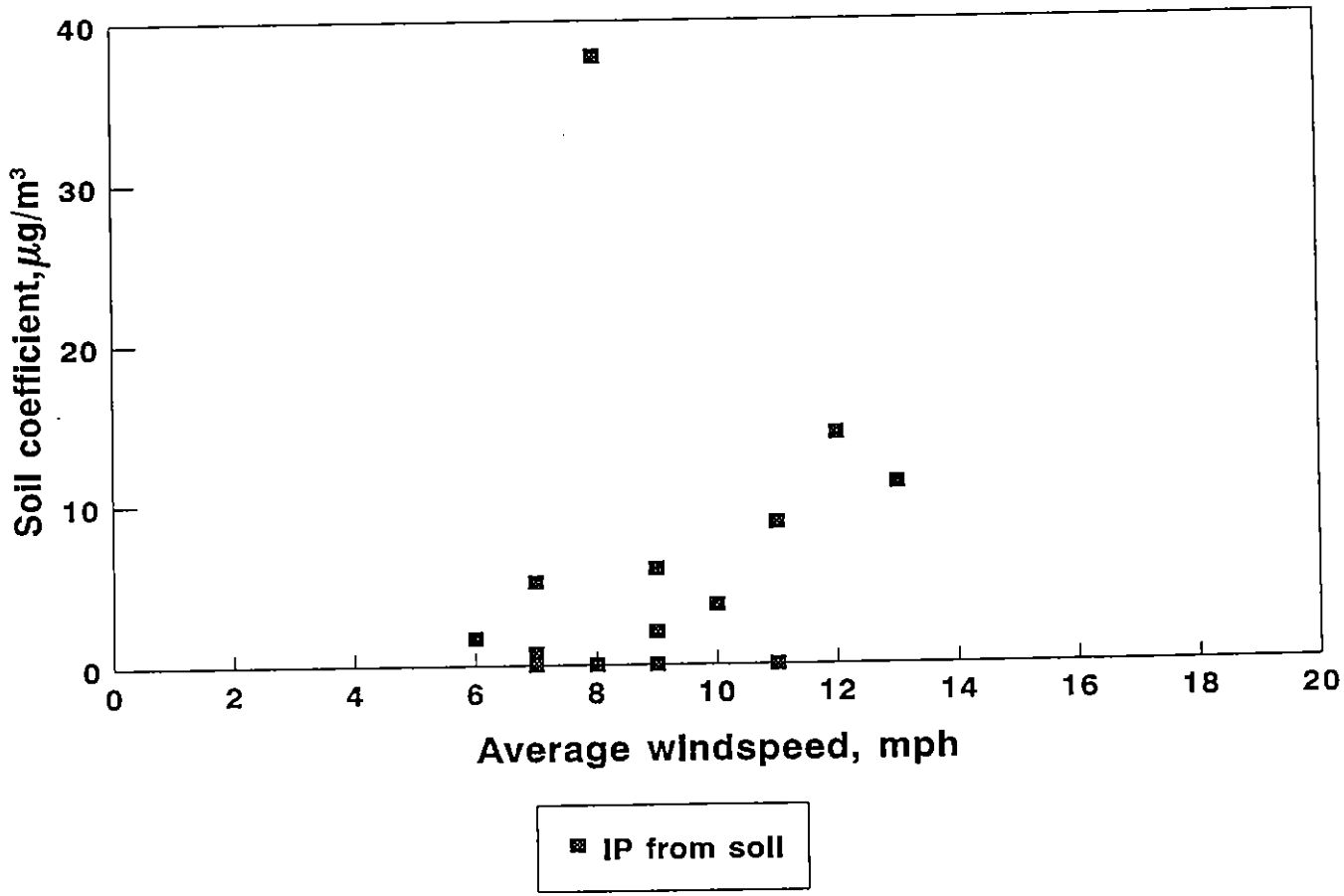
See Insert: Windspeed and Soil Coefficient

2.c. Comparison With Other Parameters

See Insert : Chicago, 1990-1991: Comparison of soil PM_{10} + NMOG with ambient silicon.

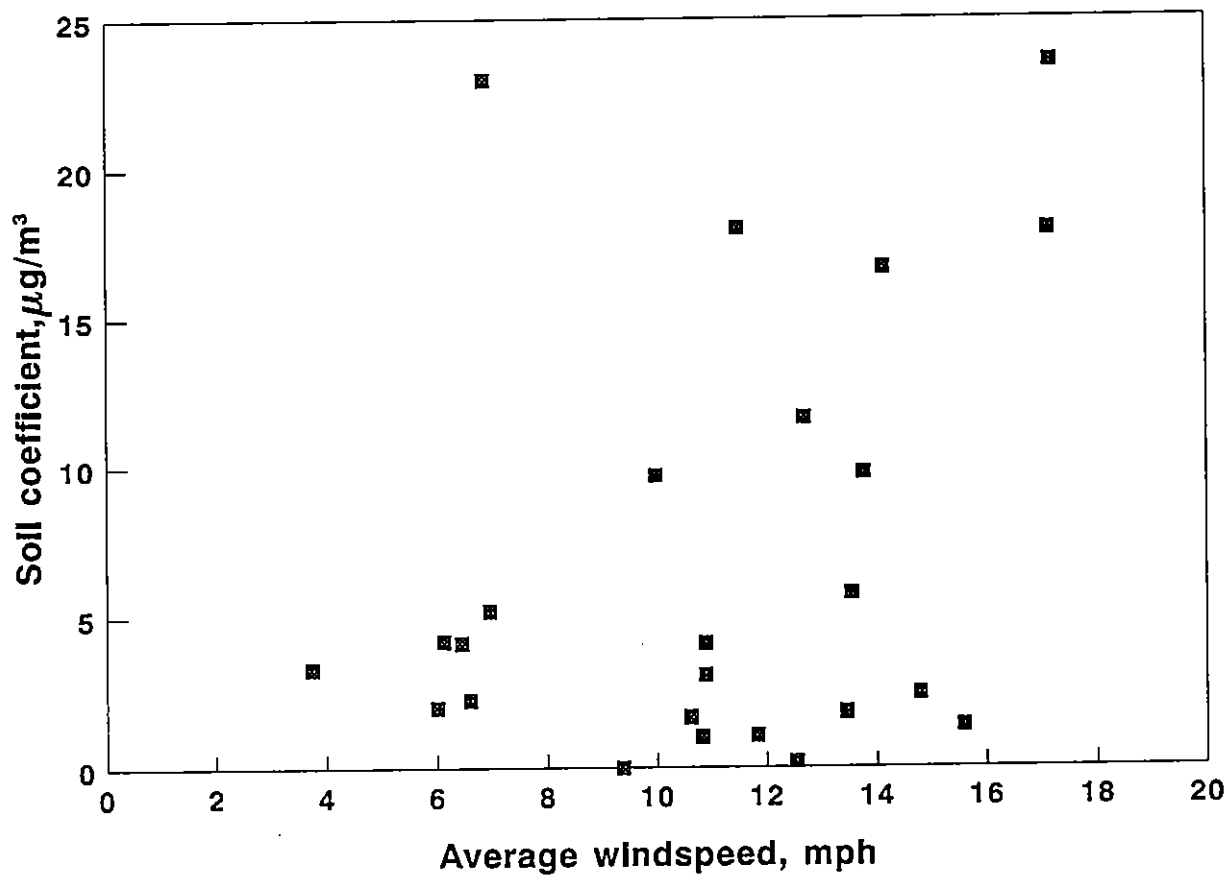
CMB Validation - Comparison with Related Parameters

Windspeed and Soil Coefficient
(Based on elemental particle composition by x-ray fluorescence)
(17 24-hour inhalable particle samples collected in Chicago at IIT during 1984)

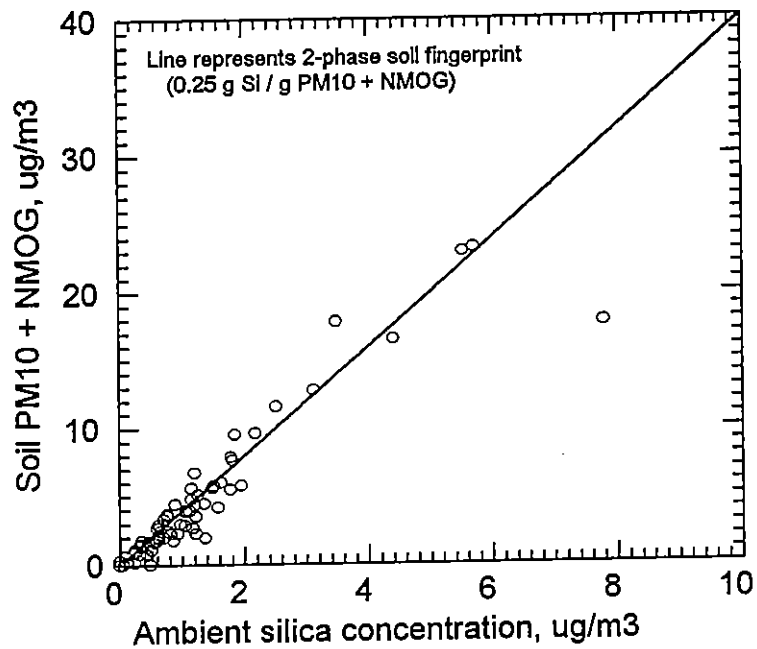


CMB Validation - Comparison with Related Parameters

Windspeed and Soil Coefficient
(Based on elemental particle composition, CO, total S, and total N)
(25 12-hour PM_{10} day-time samples collected in Chicago during Spring, Summer and Fall, 1990)



CMB Validation - Comparison with Related Parameters



Chicago, 1990-1991: Comparison of soil PM_{10} + NMOG with ambient silicon.

2.c. Comparison With Other Parameters

See Insert: Chicago, 1990-1991: Distribution of day-time diesel engine concentrations by day of the week.

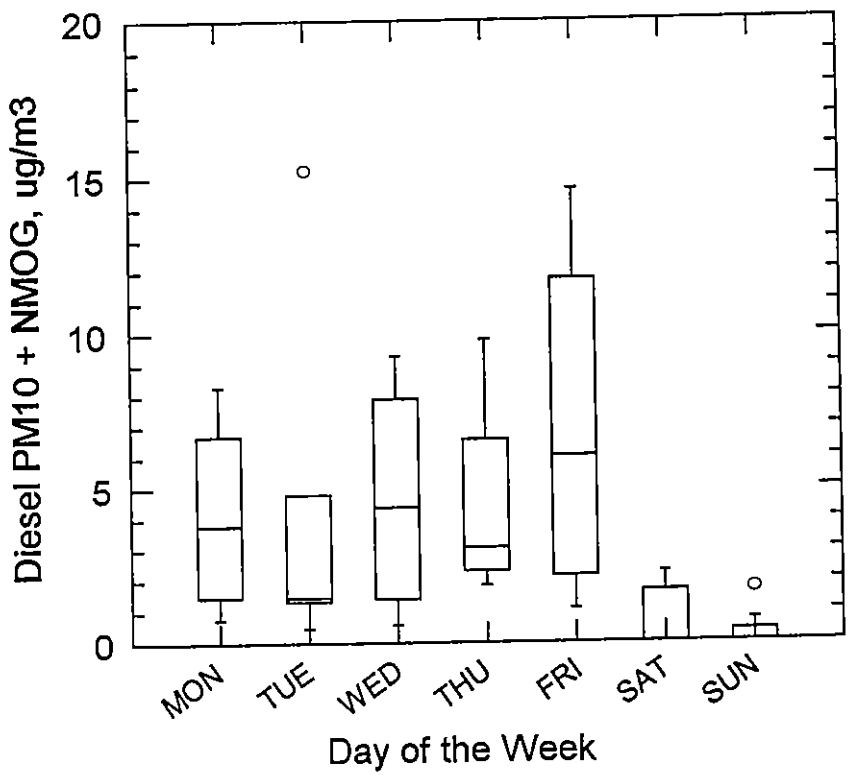
2.c. Comparison With Other Parameters

See Insert : Chicago, 1990-1991: Comparison of PM_{10} + NMOG single-phase models for vehicles.

2.c. Comparison With Other Parameters

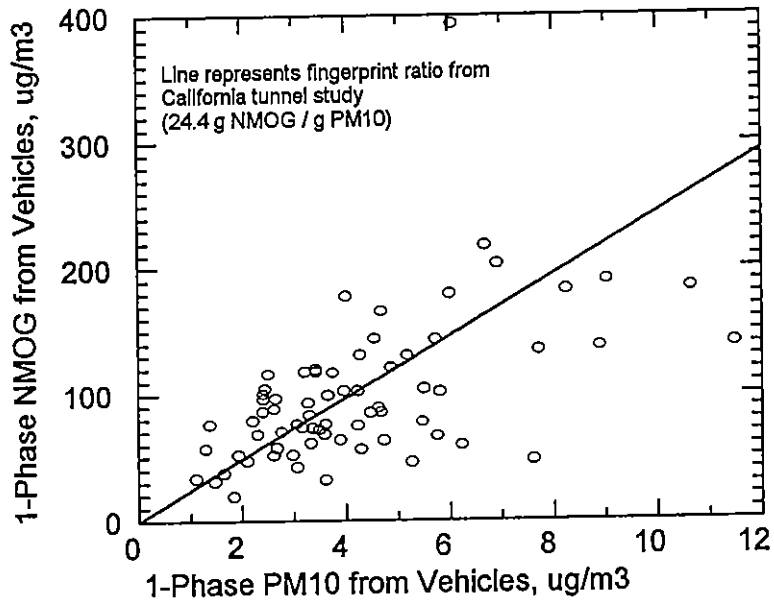
See Insert : Chicago, 1990-1991: Comparison of Mobile PM_{10} + NMOG with ambient total NO_x.

CMB Validation - Comparison with Related Parameters



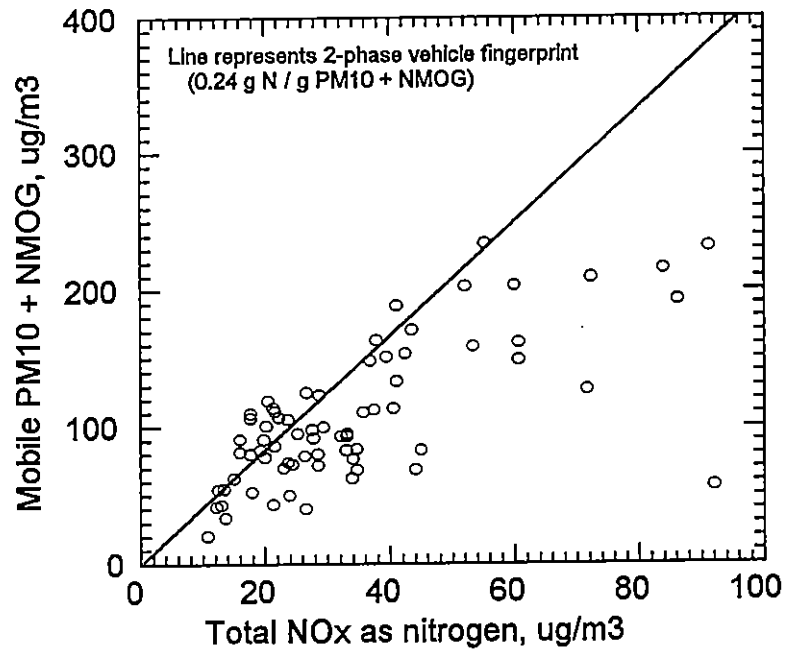
Chicago, 1990-1991: Distribution of day-time diesel engine concentrations by day of the week.

CMB Validation - Comparison with Related Parameters



Chicago, 1990-1991: Comparison of PM_{10} and NMOG single-phase models for vehicles.

CMB Validation - Comparison with Related Parameters



Chicago, 1990-1991: Comparison of Mobile PM_{10} + NMOG with ambient total NO_x.

3. CMB/Diffusion Model SIP Development Reconciliation

U.S. EPA
Office of Air Quality
Planning and Standards

1. PM_{10} SIP Development Guideline, EPA-45-/2-86-001, June 1987.

3. CMB/Diffusion Model SIP Development Reconciliation

2. Protocol for Reconciling Differences Among Receptor and Dispersion Models, EPA-450/4-87 008, March 1987.

3. PM_{10} SIP Development Guideline: Supplement, June 1988.

4. Response to Questions Regarding PM10 State Implementation Plan (SIP) Development, June 1988.

3. CMB/Diffusion Model SIP Development Reconciliation

Basic approach is still to examine air quality across the State, delineate areas where air quality needs improvement, determine the degree of improvement necessary, inventory the sources contributing to the problem, develop a strategy to reduce emissions from contributing sources enough to attain the NAAQS, implement the strategy, take the steps necessary to ensure the NAAQS are not violated in the future.

3. CMB/Diffusion Model SIP Development Reconciliation

- Best approach with respect to using chemical mass balance (CMB) is to develop control strategy which uses receptor models in conjunction with dispersion models. [PM_{10} Development Guideline]

3. CMB/Diffusion Model SIP Development Reconciliation

....the impact of specific individual sources within an air shed containing multiple sources of the same type may not be really identifiable except on wind directional samples or by a dispersion model.

3. CMB/Diffusion Model SIP Development Reconciliation

8 Step Protocol

1. Compare CMB and DM results - need minimum of 5 samples/quarter to compare with NAAQS; pick sampling days or a subset of CMB samples to be representative of DM conditions; need to group DM conditions; adjust DM with "background" concentrations; "eclectic pollution rose"

3. CMB/Diffusion Model SIP Development Reconciliation

2. Verify input data in both models and rerun if necessary

3. Recompare results

4. Refine CMB model inputs

3. CMB/Diffusion Model SIP Development Reconciliation

5. Recompare results

6. Refine dispersion model inputs and rerun

7. Recompare results and evaluate dispersion model

3. CMB/Diffusion Model SIP Development Reconciliation

8. Final model estimates as basis for control strategy - but use the model which gives the best results

3. CMB/Diffusion Model SIP Development Reconciliation

"eclectic pollution rose" - pollution rose, developed by compositing the data from several monitors surrounding the urban area, which reflects concentrations only when the wind is blowing into the urban area

3. CMB/Diffusion Model SIP Development Reconciliation

"The effective variance least squares solution is more valid than the ordinary (weighted)least squares solution only if the precision of the source data are known. Such data are often missing or of poor quality."

3. CMB/Diffusion Model SIP Development Reconciliation

P.29, Receptor Model Technical Series. Volume 5. Source Apportionment Techniques and Considerations in Combining Their Use, EPA-450/4-84-020, July 1984.

3. CMB/Diffusion Model SIP Development Reconciliation

- Example of model reconciliation

Reconciliation of ISCST Dispersion Model and CMB Receptor Model TSP Lead Apportionments Calculated Near a Primary Lead Smelter in East Helena, Montana, Patterson and Brian, AWMA Paper 92-103.01, Kansas City, 1992.

3. CMB/Diffusion Model SIP Development Reconciliation

- **East Helena out of compliance with respect to NAAQS Pb standard of 1.5 ug/m^3 on quarterly basis.**
- **Evaluated and reconciled CMB/Diffusion Model (DM) differences based on 25 highest measured daily Pb at each of 2 locations in the 3rd and 4th quarters of 1990.**

3. CMB/Diffusion Model SIP Development Reconciliation

- Selected 30% uncertainty for DM estimates; one standard error of the estimate of source coefficient for the CMB
- Compared 22 source categories

3. CMB/Diffusion Model SIP Development Reconciliation

- Criterion for reconciliation was whether intervals of uncertainty for average source contributions calculated by different models overlapped. Comparison was made on the basis of each source category.

3. CMB/Diffusion Model SIP Development Reconciliation

East Helena Pb Concentrations, ug/m^3

Rank	Firehall Site	Old Railroad Site
1	9.35	20.57
2	8.79	5.67
3	7.89	3.85
4	7.22	3.42
5	7.21	2.84

3. CMB/Diffusion Model SIP Development Reconciliation

East Helena Pb Concentrations, ug/m^3

Rank	Firehall Site	Old Railroad Site
-	-	-
-	-	-
-	-	-
25	4.42	1.44

3. CMB/Diffusion Model SIP Development Reconciliation

- Original comparison indicated only 15 of 22 source categories were reconciled for Firehall site and 18 of 22 at Old Railroad site.
- Based on these results, input data were refined for both models.

3. CMB/Diffusion Model SIP Development Reconciliation

Some of these for the ISCST model

- Error in receptor UTM coordinates corrected
- Dross plant roof emissions modeled to account for buoyant plume
- Corrections were made to process data used in daily emission calculations based on more detailed examination of process logs

3. CMB/Diffusion Model SIP Development Reconciliation

Some of these for CMB model

- At the Old Railroad site, the sinter storage baghouse stack was found to be the primary contributor of Pb. But the emissions inventory suggested that this source should not be a major contributor.

3. CMB/Diffusion Model SIP Development Reconciliation

Fitting of the source profile was driven by the under-explanation of the relatively high Na concentrations at this source. Later discovered that sodium carbonate as used liberally at plant. Adding a sodium carbonate profile greatly reduced Pb contribution from sinter storage baghouse.

3. CMB/Diffusion Model SIP Development Reconciliation

- Plant operations data were re-examined and sources adjusted accordingly. If a stored material not handled on a particular day, and winds were light or moderate, the profile for that material was not used in the CMB fit for that day.

3. CMB/Diffusion Model SIP Development Reconciliation

See Insert: Firehall Site Table

3. CMB/Diffusion Model SIP Development Reconciliation

Firehall Site

Source Category	Model	Initial % of Pb	Reconciled % of Pb
Sinter/Acid Dust Handling	CMB	35±18	24±19
	DM	11±3	10±3
East Helena Roads	CMB	8±1	23±6
	DM	11±3	20±6
Blast Furnace Building	CMB	14±8	10±10
	DM	4±1	9±3
Dross Plant & Bullion Building	CMB	7±10	14±8
	DM	31±9	19±6
All Modeled Sources	CMB	98.5	103.7
	DM	73.7	76.0

3. CMB/Diffusion Model SIP Development Reconciliation

See Insert: Old Railroad Site Table

3. CMB/Diffusion Model SIP Development Reconciliation

See Insert: Old Railroad Site Table

3. CMB/Diffusion Model SIP Development Reconciliation

Reconciliation Results

- **For both sites, 21 of the 22 source categories met the reconciliation criterion; and the category which didn't agree was not the major Pb contributor.**

3. CMB/Diffusion Model SIP Development Reconciliation

Old Railroad Site Source Category	Model	Initial % of Pb	Reconciled % of Pb
Sinter/Acid Dust Handling	CMB	3±32	12±27
	DM	27±8	26±8
East Helena Roads	CMB	16±4	18±5
	DM	37±11	9±3
Blast Furnace Building	CMB	9±8	7±6
	DM	4±1	6±2
Dross Plant & Bullion Building	CMB	4±15	13±12
	DM	25±8	23±7
Sinter Storage Baghouse Stack	CMB	40±7	4±7
	DM	1.3±0.4	1.1±0.3

3. CMB/Diffusion Model SIP Development Reconciliation

Old Railroad Site

Source Category	Model	Initial % of Pb	Reconciled % of Pb
All Modeled Sources	CMB	101.9	97.6
	DM	122.8	110.3

3. CMB/Diffusion Model SIP Development Reconciliation

- For the Firehall site, 24% of the Pb still remains unaccounted for by the Diffusion Model.

- Both models predicted the same top three categories which contributed the most Pb to each site.

Lesson XIII

CMB Model Applications:
Description of Homework Data Sets
Peter Scheff

INTRODUCTION TO RECEPTOR MODELING

Lesson Title: CMB Model Applications: Description of Homework Data Sets
Lesson: XIII
Prepared By: P.A. Scheff
Date: February 12, 1998

Lesson Goal: The goal of this lesson is to describe the data sets which will be used for the completion of the homework assignments.

Lesson Objectives: At the completion of this lesson students will be able to:

Explain the requirements for completing and submitting the homework assignments.

Explain the contents of the homework test data sets.

Explain how to get help when working on their homework assignments.

Lesson XIII. CMB Model Applications: Description of Homework Data Sets.

Peter A. Scheff
University of Illinois at Chicago

Homework Data Sets

1. **Portland Aerosol Characterization Study (PACS).**

2. **Volatile Organic Compounds in Mexico City, 1993.**

Homework Data Sets

3. **Photochemical Assessment Monitoring Station VOC data for Chicago, 1994.**

4. **Florida Atmospheric Mercury Source Apportionment Study.**

Description of Homework Data Sets

1. Portland Aerosol Characterization Study

- Data collected for CMB and State Implementation Plan development
- Six sites in Oregon
- Samples collected between 4/77 and 4/88

1. Portland Aerosol Characterization Study

- 24-hr, 8-hr and 4-hr samples for two size ranges:

  0-2.5μm and 2.5-30.0 μm aerodynamic diameter

- Samples analyzed for mass, elements, ions and carbon.

1. Portland Aerosol Characterization Study

- CMB8 contains three selected PACS samples from

  08/07/77
  08/13/77
  01/24/78

Description of Homework Data Sets

1. Portland Aerosol Characterization Study

- PACS input file: inport.in8

SOPORT.sel
POPORT.sel
ADPORT.sel
ADPORT.TXT
PRPORT.TXT

1. Portland Aerosol Characterization Study

- PACS Source profiles included (SOPORT.sel)

1	MARIN	*	Marine aerosol
2	CDUST		Crustal dust
3	UDUST	*	Urban Dust
4	AUTPB	*	Vehicle emissions, leaded fuel

1. Portland Aerosol Characterization Study

- PACS Source profiles included (SOPORT.sel)

5	RDOIL	*	Residual oil combustion
6	VBRN1		Vegetative burning
7	VBRN2		Vegetative burning
8	KRAFT	*	Kraft recovery furnace
9	SULFT		Sulfite recovery boiler

1. Portland Aerosol Characterization Study

- PACS Source profiles included (SOPORT.sel)

10	HOGFU		Wood-fired (hogged fuel) boiler
11	ALPRO	*	Aluminum processing
12	STEEL	*	Steel furnace
13	FERMN	*	Ferromanganese furnace
14	CARBO		carborundum (silicon carbide) manufacturing

1. Portland Aerosol Characterization Study

- PACS Source profiles included (SOPORT.sel)

15	GLASS	glass furnace
16	CARBF	Calcium carbide furnace
17	SO4	Single component sulfate source
18	NO3	Single component nitrate source
19	OC	Single component organic carbon source
20	EC	Single component elemental carbon source

1. Portland Aerosol Characterization Study

- PACS Fitting Species

Total		Total Mass by Gravimetry
F		Water-Soluble Fluoride by Anion Chromatography
Na	*	Sodium by Short-lived Neutron Activation
Mg	*	Magnesium by Short-lived Neutron Activation

1. Portland Aerosol Characterization Study

- PACS Fitting Species

Al	*	Aluminum by X-Ray Fluorescence
Si	*	Silicon by X-ray Fluorescence– marker for dust.
S		Sulfur by X-ray Fluorescence
Cl	*	Chlorine by X-ray Fluorescence
K	*	Potassium by X-ray Fluorescence

1. Portland Aerosol Characterization Study

- PACS Fitting Species

Ca	*	Calcium by X-ray Fluorescence
Ti	*	Titanium by X-ray Fluorescence
V	*	Vanadium by X-ray Fluorescence
CR	*	Chromium by X-ray Fluorescence
Mn	*	Manganese by X-ray Fluorescence

1. Portland Aerosol Characterization Study

- PACS Fitting Species

Fe	*	Iron by X-ray Fluorescence
Ni	*	Nickel by X-ray Fluorescence
Cu	*	Copper by X-ray Fluorescence
Zn	*	Zinc by X-ray Fluorescence
Br	*	Bromine by X-ray Fluorescence
Pb	*	Lead by X-ray Fluorescence

Description of Homework Data Sets

1. Portland Aerosol Characterization Study

- PACS Fitting Species

OC	*	Organic Carbon by Thermal/Optical Reflectance
EC	*	Elemental Carbon by Thermal/Optical Reflectance
SO4	*	Sulfate by Anion Chromatography
NO3	*	Nitrate by Anion Chromatography

1. Portland Aerosol Characterization Study

- PACS ambient sample selection file

PACS1	08/13/77	24	0	FINE	1.0	1.0
PACS1	08/13/77	24	0	COARS		
PACS2	01/24/78	24	0	FINE	2.0	2.0
PACS2	01/24/78	24	0	COARS		
PACS3	08/07/77	24	0	FINE	3.0	3.0
PACS3	08/07/77	24	0	COARS		

2. Volatile Organic Compounds in Mexico City, 1993

- Nine samples collected on three days during March of 1993 by USEPA

- 6 to 9 am sample collection in canisters (EPA method TO-14)

Description of Homework Data Sets

2. Volatile Organic Compounds in Mexico City, 1993

- High-resolution GC/FID evaluation for C2 through C13 hydrocarbons
- Sample locations:

Xalostoc	Industrial northern section of city

2. Volatile Organic Compounds in Mexico City, 1993

- Sample locations:

Merced	Center of city, high vehicle emissions
Pedregal	Southern city, residential neighborhood

2. Volatile Organic Compounds in Mexico City, 1993

- Daily mean temperatures ranged from 18 to 20°C on sample collection days.
- All monitoring sites had co-located Nox instruments

2. Volatile Organic Compounds in Mexico City, 1993

- INMEXVOC.in8 file

somexvoc.sel
pomexvoc.sel
admexvoc.sel
admexvoc.car
prmexvoc.car

2. Volatile Organic Compounds in Mexico City, 1993

- ADMEXVOC.SEL ambient sample selection file

MERCED	3/25/93	03	06	TVOC
MERCED	3/26/93	03	06	TVOC
MERCED	3/27/93	03	06	TVOC

2. Volatile Organic Compounds in Mexico City, 1993

- ADMEXVOC.SEL ambient sample selection file

PEDREGAL	3/25/93	03	06	TVOC
PEDREGAL	3/26/93	03	06	TVOC
PEDREGAL	3/27/93	03	06	TVOC

2. Volatile Organic Compounds in Mexico City, 1993

- ADMEXVOC.SEL ambient sample selection file

XALOSTOC	3/25/93	03	06	TVOC
XALOSTOC	3/26/93	03	06	TVOC
XALOSTOC	3/27/93	03	06	TVOC

2. Volatile Organic Compounds in Mexico City, 1993

- Source profiles included in SOMEXVOC.SEL

1	VEHICLES	*	VEHICLE EMISSIONS
2	GASVAPOR	*	GASOLINE VAPORS
3	LIQGAS	*	LIQUID GASOLINE
4	LPG	*	LIQUEFIED PETROLEUM GAS (Mexican Fingerprint)

2. Volatile Organic Compounds in Mexico City, 1993

See Insert: 141species identified in POMEVOC.SEL

- 141 species identified in POMEXVOC.SEL

TVOC, ETHYLENE, ACETYLENE, ETHANE, PROPYLENE, PROPANE, METHYL CHLORIDE, ISOBUTANE, VINYLCHLORIDE, 1-BUTENE, 1,3-BUTADIENE, N-BUTANE, T-2-BUTENE, C-2-BUTENE, 1,2-BUTYNE, 3-METHYL-1-BUTENE, ISOPENTANE, 1-PENTENE, 2-METHYL-1-BUTENE, N-PENTANE, ISOPRENE, T-2-PENTENE, C-2-PENTENE, VINYLDICHLORIDE, 2-METHYL-2-BUTENE, DICHLOROETHANE, FREON-113, 2,2-DIMETHYLBUTANE, CYCLOPENTANE, 4-METHYL-1-PENTENE, CYCLOPENTANE, 2,3-DIMETHYLBUTANE, MTBE, 2-METHYLPENTANE, 3-METHYLPENTANE, 2-METHYL-1-PENTENE, 1-HEXENE, cis-1,2-DICHLOROETHYLENE, N-HEXANE, T-3-HEXENE, T-2-HEXENE, C-2-HEXENE, ETBE, 2,2-DIMETHYLPENTANE, METHYLCYCLOPENTANE, 2,4-DIMETHYLPENTANE, 2,2,3-TRIMETHYL-1-BUTENE, 2,2,3-TRIMETHYLBUTANE, C-4,4-DIMETHYL-2-PENTENE, 2,4-DIMETHYL1-PENTENE, BENZENE, 3,3-DIMETHYLPENTANE + CARBON-TETRACHLORIDE, 3,3-DIMETHYL-1-HEXENE, CYCLOHEXANE, 4-METHYL-1-HEXENE, 2-METHYLHEXANE, 2,3-DIMETHYLPENTANE, 3-METHYLHEXANE, 1,2-DICHLOROPROPANE, 1-C-3-DIMETHYLCYCLOPENTANE, 3-ETHYLPENTANE, 2,2,4-TRIMETHYL-1-PENTENE, N-HEXANE, 2,4,4-TRIMETHYL-1-PENTENE, METHYLCYCLOHEXANE 2,5-DIMETHYLHEXANE, 2,4-DIMETHYLHEXANE, 3&4-METHYLCYCLOHEXANE, 1,1,2-TRICHLOROETHANE, 2,3,4-TRIMETHYLPENTANE, TOLUENE, 2,3-DIMETHYLHEXANE, 2-METHYL-3-ETHYLPENTANE, 2-METHYLHEPTANE, 4-METHYLHEPTANE, 3-METHYLHEPTANE, 2,2,5-TRIMETHYLPENTANE, 1-OCTENE, 1,1-DIMETHYLCYCLOHEXANE, T-4-OCTENE, T-3-OCTENE, CYCLOHEPTANE, N-OCTANE, 1-T-2-DIMETHYLCYCLOHEXANE, PERCHLOROETHYLENE, 2,3,5-TRIMETHYLHEXANE, 2,2-DIMETHYLHEPTANE, 2,4-DIMETHYLHEPTANE, 4,4-DIMETHYLHEPTANE, 2,6-DIMETHYLHEPTANE, CHLOROBENZENE, 2,5-DIMETHYLHEPTANE, 3,3-DIMETHYLHEPTANE, ETHYLBENZENE, M&P-XYLENE, 4-METHYLOCTANE, 3-METHYLOCTANE, STYRENE, O-XYLENE&1,1,2,2-TETRACHLOROETHANE, 1-NONENE, N-NONANE, I-PROPYLBENZENE, 4,4-DIMETHYLOCTANE, CYCLOOCTENE, ISOPROPYLBENZENE, 4,4-DIMETHYLOCTANE, CYCLOOCTANE, 2,6-DIMETHYLOCTANE, A-PINENE, N-PROPYLBENZENE, M-ETHYLTOLUENE, 2,3-DIMETHYLOCTANE, 5-METHYLNONANE, 1,3,5-TRIMETHYLBENZENE, 2-METHYLNONANE, 3-METHYLNONANE, O-ETHYLTOLUENE, 1-DECENE, 1,2,4-TRIMETHYLBENZENE, T-BUTYLCYCLOHEXANE, N-DECANE & M-DICHLOROBENZENE, P-DICHLOROBENZENE, SEC-BUTYLBENZENE, 1,2,3-TRIMETHYLBENZENE, 0-DICHLOROBENZENE, N-BUTYLCYCLOHEXANE, 1,3-DIETHYLBENZENE, N-BUTYLBENZENE, 1,3-DIMETHYL-4-ETHYLBENZENE, 4-T-BUTYLTOLUENE, N-UNDECANE
1,2,4,5-TETRAMETHYLBENZENE, 1,2,3,5-TETRAMETHYLBENZENE, M-DIISOPROPYLBENZENE, 1,2,3,4-TETRAMETHYLBENZENE, 2,4,6-TRIMETHYLSTYRENE, NAPTHALENE & N-1-DODECENE, N-DODECANE, HEXACHLOROBUTADIENE, N-1-TETRADECENE, N-TRIDECANE, N-TETRADECANE

2. Volatile Organic Compounds in Mexico City, 1993

TNMHC and NOx concentrations in Mexico City

Date	Location	TNMHC ppmC	NOx ppm	RATIO
3/25	Xalostoc	5.88	0.348	16.9
3/26	Xalostoc	6.65	0.349	19.0
3/27	Xalostoc	5.47	0.342	16.0

2. Volatile Organic Compounds in Mexico City, 1993

Date	Location	TNMHC ppmC	NOx ppm	RATIO
3/25	Merced	3.99	0.163	24.5
3/26	Merced	3.42	0.165	20.8
3/27	Merced	6.01	0.226	26.6
3/25	Pedregal	1.16	0.134	8.3
3/26	Pedregal	2.58	0.178	14.5
3/27	Pedregal	1.08	0.057	19.0

3. Photochemical Assessment Monitoring Station Data

- **Type 2 PAMS station located in downtown Chicago**
- **3-hour samples starting at 0:00, 6:00, 12:00 and 15:00**

3. Photochemical Assessment Monitoring Station Data

- Samples collected every third day
- Monitoring site had co-located Nox instrument

3. Photochemical Assessment Monitoring Station Data

- INCHIVOC.in8 file

SOCHIVOC.SEL
POCHIVOC.SEL
ADCHIVOC.SEL
ADCHIVOC.CAR
PRCHIVOC.CAR

3. Photochemical Assessment Monitoring Station Data

- ADCHIVOC.SEL ambient sample selection file

NW	6/7/94	3	0	TVOC
NW	6/7/94	3	6	TVOC
NW	6/7/94	3	12	TVOC
NW	6/7/94	3	15	TVOC

3. Photochemical Assessment Monitoring Station Data

- ADCHIVOC.SEL ambient sample selection file

NW	7/13/94	3	0	TVOC
NW	7/13/94	3	6	TVOC
NW	7/13/94	3	12	TVOC
NW	7/13/94	3	15	TVOC

3. Photochemical Assessment Monitoring Station Data

- ADCHIVOC.SEL ambient sample selection file

NW	8/8/94	3	0	TVOC
NW	8/8/94	3	6	TVOC
NW	8/8/94	3	12	TVOC
NW	8/8/94	3	15	TVOC

3. Photochemical Assessment Monitoring Station Data

- Source profiles included in SOCHIVOC.SEL

1	VEHICLES	*	VEHICLE EMISSIONS
2	GASVAP	*	GASOLINE VAPORS
3	WHOLE	*	WHOLE GASOLINE
4	REFINE	*	PETROLEUM REFINERY EMISSION

3. Photochemical Assessment Monitoring Station Data

5	GRAPHART	*	GRAPHIC ARTS
6	ARCHCOAT	*	ARCHITECTURAL COATING
7	COKE	*	COKE OVENS
8	CNG	*	COMMERCIAL NATURAL GAS
9	LPG	*	LIQUID PETROLEUM GAS (US fingerprint)

3. Photochemical Assessment Monitoring Station Data

See Insert: 52 species identified in POCHIVOC.SEL

4. Florida Atmospheric Mercury Source Apportionment Study

- Samples were collected in South Florida, Aug-Sept 1995.
- Ambient data is from 5 sites collected primarily at 12 hour interval 8am-8pm-8am.
- The background site was Adams Key.

- 52 species identified in POCHIVOC.SEL

TVOC, ETHYLENE, ACETYLENE, ETHANE, PROPYLENE, PROPANE, ISOBUTANE, 1-BUTENE, N-BUTANE, T-2-BUTENE, C-2-BUTENE, 3-METHYL-1-BUTENE, ISOPENTANE, 1-PENTENE, N-PENTANE, ISOPRENE, T-2-PENTENE, C-2-PENTENE, 2-METHYL-2-BUTENE, 2,2-DIMETHYLBUTANE, CYCLOPENTANE, 4-METHYL-1-PENTENE, 2,3-DIMETHYLBUTANE, 3-METHYLPENTANE, 2-METHYL-1-PENTENE, N-HEXANE, T-2-HEXENE, C-2-HEXENE, METHYLCYCLOPENTANE, 2,4-DIMETHYLPENTANE, BENZENE, CYCLOHEXANE, 2-METHYLHEXANE, 2,3-DIMETHYLPENTANE, 3-METHYLHEXANE, METHYLCYCLOHEXANE, 2,3,4-TRIMETHYLPENTANE, TOLUENE, 2-METHYLHEPTANE, 3-METHYLHEPTANE, N-OCTANE, ETHYLBENZENE, M&P-XYLENE, STYRENE, O-XYLENE & 1,1,2,2-TETRACHLOROETHANE, N-NONANE, ISOPROPYLBENZENE, N-PROPYLBENZENE, 1,3,5 & 1,2,4-TRIMETHYLBENZENE, CYCLOPENTENE, 2-METHYLPENTANE, 2,2,4-TRIMETHYLPENTANE, N-HEPTANE, NOX

4. Florida Atmospheric Mercury Source Apportionment Study

- The Flag site was in Broward county 5km from a large incinerator and 8km from the Everglades oil fired power plant FT Lauderdale. The THP site was nearest the Everglades, the IND and MNS sites were in Dade County.

4. Florida Atmospheric Mercury Source Apportionment Study

- The incinerator profiles were from the Dade county energy recovery incinerator, a medical waste incinerator few miles east of the Dade incinerator and a cement Kiln using coal as a fuel.

4. Florida Atmospheric Mercury Source Apportionment Study

- Both INNA and XRF data are included in the ambient and source profiles.

- Source profile file: PRSOFAM7.txt
- Ambient data file: ADSOFAM7.txt