



Quality Assurance Enhancements to the SMOKE Modeling System

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**Emission Inventory Conference:
One Atmosphere, One Inventory,
Many Challenges**

May 1 – 3, 2001



Acknowledgements

- U.S. EPA OAQPS funding
- Thanks for feedback from
 - Norm Possiel
 - Pat Dolwick
 - Greg Stella
 - Bill Benjey



Overview

- **SMOKE summary**
- **Quality issues and strategies**
- **New SMOKE quality assurance**
 - Synopsis
 - Report configuration “language”
 - Report examples (input and output)
- **1996 NEI application**
- **Future directions**



SMOKE Summary (1)

- **Emissions modeling system for preparing model-ready inputs**
- **Supports a variety of AQMs for ozone and PM modeling**
- **Processes area, biogenic, on-road and non-road mobile, and point sources**
- **Temporal allocation, chemical speciation, and grid cell allocation**
- **Efficient emissions processing algorithms (sparse matrix)**



SMOKE Summary (2)

- Version 1.3 integrated with Models-3
- Benefits
 - Fast and smaller file sizes
 - Does not rely on third party software
- Shortcomings of version 1.2
 - Input data preparation
 - **Quality assurance**
 - Growth and controls



Data Quality Issues

- **Data from many sources needs to be checked for consistency**
- **Hundreds of thousands of emissions sources for regional modeling domains**
- **Missing data and bad values**
- **Input errors for temporal allocation, chemical speciation, grid cell assignments, and other steps**



Quality Assurance Strategies

- Automated input file quality and format checking
- Automated checking for use of default profiles
- **Reports at many levels of detail for manual inspection of data values and emissions processing**
- Prioritizing emissions data by emissions magnitude
- Comparison to PAMS data
- Visualization



Synopsis of New SMOKE Quality Assurance

- **Smkreport program provides flexible tabular reporting tool**
- **Report configuration “language” tailored to emissions**
- **Intelligent defaults and preset reports**
- **Outputs**
 - **Formatted for input to spreadsheet**
 - **Automatic headers**
 - **Metadata including input instructions**



Report Configuration Language

- Any processing steps can be optionally applied to emissions values in report
- Control pollutants, species, and units
- Control columns included in report
 - e.g. SCC, cell, stack parameters, emissions
- Control basis of summary emissions
- Apply source grouping
- Control number of reports per file



Example 1: State and county report with daily totals

- **Input instructions**

```
/NEWFILE/ /mydir/smoke/myreport.txt  
/CREATE REPORT/  
TEMPORAL  
BY STATE NAME  
BY COUNTY NAME  
/END/
```

- **Outputs**

- Headers
- Columns for date, state name, county name, and emissions of inventory pollutants
- Metadata



Example 2: SCC and county report, after gridding

```
/CREATE REPORT/  
GRIDDING  
BY SCC10  
BY COUNTY  
/END/
```

● Notes

- Left off NEWFILE packet this time
- SCC10 only currently allowed
- No NAME used with county this time



Example 3 (part 1): Using a region group and reporting by surrogates type

```
/DEFINE GROUP REGION/ NC w/o Triangle
INCLUDE
37000      ## NC state code
EXCLUDE
37063      ## Durham Co
37135      ## Orange Co
37183      ## Wake Co
/END/
```



Example 3 (part 2): Using a region group and reporting by surrogates type

```
/CREATE REPORT/  
TITLE NC area sources w/o RTP counties  
SELECT REGION NC w/o triangle  
BY COUNTY NAME  
BY SRGCODE  
/END/
```

● Notes

- Group labels are not case sensitive
- BY SRGCODE causes emissions to be aggregated by surrogate code



Example 4: Using an in-line subgrid and reporting by cell, source, and elevated status

```
/CREATE REPORT/  
SELECT SUBGRID (100,23) TO (101,24)  
BY CELL  
BY SOURCE STACKPARAM NAME  
BY ELEVSTAT  
/END/
```

● Notes

- Subgrids can also be defined with a /DEFINE SUBGRID/ packet
- STACKPARAM and NAME are optional
- GRIDDING implied with BY GRID



Example 5: Reporting hourly emissions before speciation and summed after speciation

```
/CREATE REPORT/  
BY HOUR  
BY STATE NAME  
SPECIATION  
SELECT DATA VOC S-VOC  
/END/
```

● Notes

- **SELECT DATA** instruction used for specifying emissions to include
- Default includes all pollutants and (when appropriate) species



Other Instructions

- **BY ROADCLASS**
- **NUMBER**
 - To set format of emissions fields (e.g., the number of decimal places and scientific)
- **UNITS**
 - To set the units used in the reports



1996 NEI Application

- **Version 3.11 of NEI**
- **U.S. national 36-km grid**
- **Relied on summary reports such as state, SCC, and state/SCC**
- **Used more specific reports when summary reports raised questions**
- **Examples of specific problems:**
 - **Wildfire emissions in NV**
 - **Elevated point sources for investigating a plume rise issue**



Future QA Directions

- **Increased use and capabilities of Java Analysis and Reporting Tool (JART)**
- **Natural extensions to Smkreport**
 - Additional group types
 - Additional BY types
- **PAMS analyses**



Future SMOKE Directions

- **MOBILE6**
- **Emissions factor importing**
- **Toxics (ASPEN, REMSAD, ISCST3)**
- **Include uncertainty estimates in emissions processing**



More Information

<http://envpro.ncsc.org/products/smoke>