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Quality Assurance Enhancements to the SMOKE Modeling System

Marc Houyoux and Zac Adelman

MCNC – Environmental Programs
mhouyoux@mcnc.org

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One Atmosphere, One Inventory,
Many Challenges**

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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**

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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)**

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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**

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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**

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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**

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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**

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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**

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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**

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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/
```

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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**

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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 STACKPARM NAME
BY ELEVSTAT
/END/
```

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

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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**

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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**

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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**

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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**

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Future SMOKE Directions

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