

ABSTRACT

We processed the National Emissions Inventory 96 (NEI96) version 3.11 through version 1 of the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. Using an IBM RS/6000 supercomputer, we prepared emissions for a Community Multiscale Air Quality (CMAQ) modeling system study of ozone and particulate matter over the United States and Canada for the entire year of 1996. For quality assurance, we compared the processed inventory to the NEI96 database totals and performed qualitative spatial analyses using the Package for Analysis and Visualization of Environmental data (PAVE). In addition to summaries of SMOKE performance in processing the NEI96 version 3.11, we present a technique for executing large SMOKE applications.

Processing the National Emissions Inventory 96 (NEI96) version 3.11 with SMOKE*

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METHODS

We used an execution-based SMOKE scripting procedure to accommodate this large, data-intensive application. Viewing SMOKE execution by the number of times that an individual module is implemented, rather than by source category, allows for a more quality-assured emissions generation process. The traditional method of organizing emissions processing by source category leads to redundancy in the modeler's interaction with SMOKE. We based the SMOKE model execution for this application on three primary classes of scripts: yearly, monthly, and daily.

Figures 1 and 2 compare the source and execution based scripting techniques; Table 1 summarizes the SMOKE scripts used in this application.

Script	CPU time (hh:mm:ss)	Wall Clock time (hh:mm:ss)
Inventory	00:25:45	00:29:41
Monthly	01:56:10	02:29:13
Holiday	06:56:49	09:17:51
Daily	00:06:20	00:08:47
Total	79:17:52	103:00:55

Table 4. SMOKE computational performance statistics for a single execution of each script on an IBM RS/6000 SP2; total times reflect the time required to complete all of the annual SMOKE run. Note: times will vary depending on the number and content of QA reports.

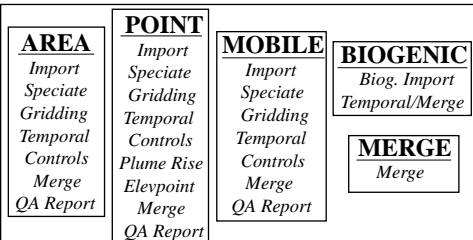


Figure 1. Conceptual model of SMOKE scripts distributed with the model (source-based).

Script	Frequency	SMOKE description
Yearly	1x/yr	Inventory import, Speciate, and Gridding for area and point. Biogenic inventory import. QA reporting for area and point
Monthly	1x/month	Inventory import, Speciate, and Gridding for mobile. Temporal for area, point, and mobile. QA reporting for area, point, and mobile
Holiday	1x/year	Temporal for area, point, and mobile
Daily	1x/day	Plume rise for point; Temporal for biogenic. Merge for all sources

Table 1. NEI 96 SMOKE scripting description used in this application.

Source	Import	Gridding	Temporal ¹	Plm.Rise ^b	Speciate	Merge ¹	Totals
Area	76.4	15.4	296.5	n/a	30.3	25.0	473.9
Point	106.6	1.6	318.0	159.0	33.4	99.8	751.8
Mobile	32.2	20.7	238.6	n/a	25.1	25.0	366.7
Biogenic	1.1	n/a	n/a	n/a	n/a	8.0	18.2
Merged	n/a	n/a	n/a	n/a	n/a	n/a	104.6
Total	217.4	37.7	853.1	159.0	177.6	165.8	

¹64 copies (4/month+16 holidays) ²365 copies

Table 2. Single-day file sizes (Mb) for U.S. NEI96, July 3, 1996. All columns are for one copy except where indicated.

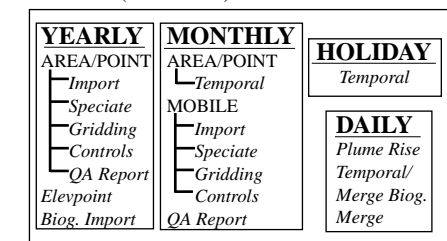


Figure 2. Conceptual model of SMOKE scripts that we used to process the annual NEI 96 inventory (execution-based).

*SMOKE is available for free on the MCNC website: <http://envpro.ncsc.org/products/smoke>

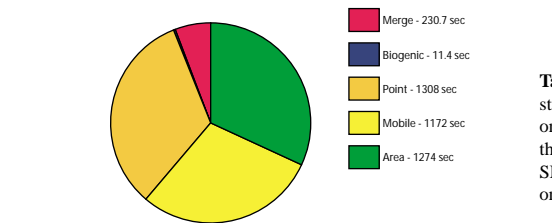


Figure 3. Relative CPU times for SMOKE to process a single day for each source category for the NEI 96 for the entire U.S. and Canada.

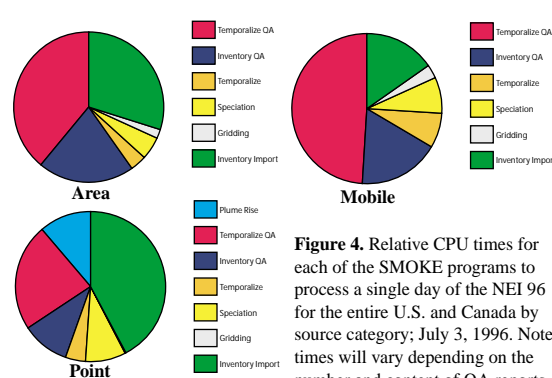


Figure 4. Relative CPU times for each of the SMOKE programs to process a single day of the NEI 96 for the entire U.S. and Canada by source category; July 3, 1996. Note: times will vary depending on the number and content of QA reports.

CONCLUSIONS

The execution-based scripts used to process the NEI96v3.11 increase the flexibility of implementing the various SMOKE programs for an annual emissions run. The new scripts simplify the management of the SMOKE data requirements and minimize the amount of modeler interaction with SMOKE. Combined with the new SMOKE QA tool, Smkreport, these scripts give emissions modelers the flexibility to generate massive emissions data sets with an almost unlimited combination of QA reports for troubleshooting problems with inventories.