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THE STATE OF THE SMOKE MODELING SYSTEM: 2001/2002

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1 OVERVIEW

Over the past 8 years, MCNC has developed the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system as part of the overall effort to built a community modeling system. This extended abstract provides a summary of the history of SMOKE, a description of current trends in emissions processing, a summary of recent SMOKE enhancements, a description of outstanding issues with the SMOKE version 1.4 beta release, a synopsis of ongoing SMOKE development work, a listing of recent SMOKE applications by MCNC, and concerns for the future of release and maintenance of the SMOKE system.

2 SMOKE STATUS TO DATE

In 1994, Dr. Carlie Coats of MCNC developed the idea for SMOKE: use vector-matrix multiplication to greatly enhance the speed of the emissions processing needed to support North Carolina's air quality modeling efforts. At that time, processing a single emissions episode with the Emissions Preprocessing System, 2.0 (EPS 2.0) took roughly 33% more CPU time and four times more overall time than it took to run the Urban Airshed Model, version IV (UAM IV). Dr. Coats started to build a prototype system that included vector-matrix processing for all steps of emissions processing. This prototype multiplied the *vector* of emissions values with a *matrix* for each set of factors needed for chemical speciation, temporal allocation, and spatial allocation.

Initially, the prototype supported many of the capabilities of the EPS 2.0 for area, biogenic, and point sources, and did so about 20 times faster. We then added the mobile-source processing that used the MOBILE5a model and included readers for input file formats of the Emissions Modeling System, 95 (EMS95). The SMOKE prototype was tested on inventories from the North Carolina Department of Environment and Natural Resources (NC DENR) and the Ozone Transport and Assessment Commission. Since that time, SMOKE has been applied in dozens of major air quality modeling efforts, has been integrated with the Models3 system to create SMOKE version 1, has been also integrated with the Multimedia Integrated Modeling System (MIMS), and has most recently been released as SMOKE version 1.4 beta in May of 2002.

3 CURRENT TRENDS IN EMISSIONS MODELING

Over the past year, several major trends in emissions modeling have formed or have been perpetuated. First, EPA has continued processing annual and national emissions cases for air quality modeling in CMAQ. Second, the regional modeling centers have begun their modeling efforts, particularly the Western Regional Air Partnership (WRAP) modeling center. Like EPA's work, the WRAP emissions episodes have been annual episodes, which is necessary for proper assessment of regional haze. It seems clear that the efforts of the regional modeling centers will strongly influence the overall direction of the modeling community. Third, groups have been preparing to process or actually processing emissions for both ozone and regional haze modeling, in anticipation of the Clean Air Act (CAA) Section 308 and 309 requirements. Fourth, groups have been using MOBILE6 emissions, even using precomputed monthly MOBILE6 emission inventories in place of day-specific MOBILE5b inventories modeled with SMOKE. Fifth, I have observed an increased interest in SMOKE processing for the Statewide Air Pollutant Research Center (SAPRC) chemical mechanism, which has recently been released as part of the CMAQ modeling system. Finally, the PC-based Linux computers have become the platform-of-

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choice for EPA, states, and the regional modeling centers.

4 RECENT SMOKE ENHANCEMENTS

SMOKE continues to be improved by us at MCNC as well as by other groups. In this section, I describe improvements since the version 1.4 beta release, the updates made for the 1.4 beta release, and known problems with that release.

4.1 SMOKE improvements since the Version 1.4 beta release

The major update to SMOKE since version 1.4 beta was released is the completed integration with SMOKE and MOBILE6.2. A packaged version of this code is currently planned for public release on December 20th, 2002.

We have made several enhancements to reporting capabilities. We have updated the main reporting program, Smkreport, to be able to include growth and control adjustments to the emissions in the report. This allows for easier comparison and checking emissions before and after growth and/or controls. We also enhanced Smkreport to include SCC description for area and mobile sources when reporting by source.

The main merge program, Smkmerge, has been updated to be able to apply multiplicative controls for mobile sources.

Also, Jeff Vukovich at MCNC has added a three-dimensional sea-salt model to SMOKE. This model can be used for meteorology-based predictions of sea-salt emissions in coastal regions.

Lastly, we made several significant corrections since the version 1.4 beta release. These include:

- In Cntlmat, we corrected calculation of controls for mobile sources, including the case when vehicle-miles-traveled (VMT) data are in the inventory.
- In Smkreport, we corrected reporting by layer, corrected use of layer fractions, and added the default of "mass" speciation when no speciation type is specified.
- We corrected the I/O API for January 1st for computing temporal adjustments and including daylight savings time in October. This fixed problems in SMOKE hourly emissions for the same time periods.
- In Temporal, we fixed the PC version so that it runs without inadvertently ending.
- In Smkmerge, we corrected a problem that cased SMOKE to abort when writing ASCII elevated files. We also repaired the inadvertent dropping of emissions when more than one source shares a stack ID.

These changes have not been updated on the version 1.4 beta release on the MCNC web site, but have been used in ongoing applications of SMOKE at MCNC for various clients and at EPA.

4.2 Improvements included with version 1.4 beta release

SMOKE version 1.4 beta includes many additional features, as summarized below.

- **Inventory import.** Included coarse particulate matter (PMC) computation when also importing mobile VMT data and for ozone-season emissions values. Added import of the Continuous Emissions Monitoring (CEM) data and matching to Inventory Data Analyzer (IDA) formatted inventories. Repaired EMS-95 hour-specific implementation to support using this hour-specific format with IDA-formatted annual inventories. Updated to permit computation of "annual" emissions based on ozone-season emissions when annual emissions are needed but not provided. Corrected use of weekday normalization to apply only to inventory formats that support average-day emissions values.
- **Controls.** Updated the cross-referencing to permit assignment of controls by all four levels of partial SCCs. Repaired application of control factors when controls are pollutant-specific, and repaired generating multiple control or growth matrices in one run. Improved report formats.
- **Inventory growth/control.** Fixed inventory growth to correctly output the IDA format. Updated to be able to apply any number of growth or control matrices in one program run.
- **Elevated source selection**. Added support for user-defined selection of elevated sources based on stack parameters, emissions, emissions rank, plant ID, source ID, analytical plume rise, and any combination of these items.
- **Spatial allocation.** Updated all programs that use gridded inputs to support extraction of data from a larger grid than the SMOKE output grid. Extractions are supported for spatial surrogates, biogenic land use, and meteorology input data.
- **Temporal allocation.** For mobile sources, allowed use of the minimum and maximum temperatures for MOBILE5b from the previous day, when meteorology data were not available at the end of an episode. Corrected a bug in time zone adjustments to diurnal profiles that occurred when the output time zone exceeded the source time zone.

- **Biogenic emissions.** Released Biogenic Emission Inventory System, version 3 (BEIS3).
- **Layer fractions.** Added support of precomputed, hour-specific plume rise for WRAP wildfire modeling, including their use in UAM-style elevated point source ASCII files. We used artificial "stacks" to force emissions into the required model layers.
- **Quality Assurance.** Updated reporting to include profile codes for speciation, gridding, and temporal profiles. Added selection of inventory records based on noncontiguous subgrid, region codes, and elevated status. Added normalization of emissions by population and grid cell area.

4.3 Known problems with SMOKE version 1.4 beta release

Despite the corrections provided with the version 1.4 beta release and additional corrections made since then, there are several known additional problems worth noting here.

- **Inventory import.** The IDA input format added to work around Silicon Graphic compiler bugs has broken the IDA input format on Linux PCs. The VMT data in EMS-95 format has problems on the Sun platform. Missing values for CEM data are not handled properly. In addition, an enhancement has been requested to identify bad stack coordinates in a report.
- **Controls.** An unintended abort has been reported when running on the Sun platform.
- **Inventory growth/control.** Growth and control factors are not applied to ozone-season values.
- **Spatial allocation.** Link sources with zero-length cause an internal error, but should simply cause all emissions to be placed at the point location. Also, the MGSUP intermediate file written and used by SMOKE to report the spatial surrogates applied by source is incomplete.
- **Temporal allocation.** A user has reported a possible mistake in the temporal cross-reference files released with version 1.4 of SMOKE.
- **Biogenic emissions.** The Tmpbio program has erroneous "close" statements that get called for unused optional inputs. This can cause crashes on Sun platforms.
- **Merging.** The state/county summaries of controlled emissions have zero emissions on any pollutant, state, or county that is not controlled, instead of reporting the uncontrolled value.
- **Quality Assurance.** Smkreport is incapable of reporting the speciation profile codes when using the MOBILE5b processing approach for mobile sources.

5 ONGOING SMOKE DEVELOPMENT

SMOKE continues to be developed in a variety of ways. First, Jim Godowitch of EPA's Office of Research and Development has recently provided the CMAS with an updated plume-rise algorithm to add to SMOKE.

Second, MCNC has been working with EPA's Office of Air Quality Planning and Standards (OAQPS) to enhance SMOKE for toxic inventory processing. The first phase of this work was integration of SMOKE with MOBILE6.2 for support of criteria, particulate, and toxics mobile pollutants. MCNC is also updating SMOKE to process the 1999 nonroad toxics inventory. The combined MOBILE6.2/nonroad toxics release will be the version 1.5 beta, scheduled for release on December 20, 2002. Following these updates, OAQPS has also funded support of toxic inventories for area and point sources, which will be completed in May of 2003.

For the WRAP RMC, MCNC is also compiling SMOKE for the PC-Linux platform using the Portland Group compiler. Currently, the 1.3.2 release developed for the WRAP is performing identically on SGI and PC Linux platforms using the SMOKE demo data. We are currently testing the more complex WRAP base case inventory. We are also seeking about $12K of funding to support the final version 1.4 release, including a PC Linux version.

Over the past year, MCNC has been wrapping up a 4-year project under an EPA STAR grant with Drs. Chris Frey and Dan Loughlin at NC State University. This project has resulting in SMOKE version 1U, which has been substantially modified to support propagating uncertainty estimates of inventory emissions through SMOKE, resulting in Monte Carlo model-ready emissions data. We are currently processing 12 cases that will test the impact of inventory uncertainties on a 4-km air quality simulation over Charlotte, North Carolina. We are using the Multiscale Air Quality SImulation Platform (MAQSIP) for our air quality simulations, in coordination with modeling efforts at NC DENR. We are also working towards a journal article that we plan to submit in January of 2003.

Lastly, we will soon be starting an effort with the American Chemistry Council and Dr. Bill Carter at the University of California at Riverside. In this project, we will enhance SMOKE for dynamically creating chemical speciation profiles and supporting the SAPRC chemical mechanism.

6 RECENT SMOKE APPLICATIONS

Over the past year or so, numerous applications of SMOKE have been performed both at MCNC and elsewhere. At MCNC, we have used SMOKE to:

- support real-time ozone forecasting in the eastern U.S.;
- apply the new sea-salt model for input to CMAS in the Gulf Coast;
- develop CMAQ emission inputs in the southwestern U.S. for the Big Bend Regional Aerosol and Visibility Observation (BRAVO) study: a 1999, four-month regional modeling episode;
- develop 36-km, 12-km, and 4-km emission inventories for episodic simulations on the eastern U.S. using the SMOKE/MOBILE6 integration for mobile sources;
- develop annual and national CMAQ inputs for the Clear Skies Initiative at 36-km for base and future year efforts;
- create annual CMAQ inputs for the western U.S. with the WRAP Regional Modeling Center for a 1996 base case and several 2018 future-year cases in support of the CAA Section 309 modeling; and
- support NH_x cycling research efforts over the eastern U.S.

SMOKE is also gaining widespread use in the air quality modeling community. The following descriptions provide some examples of efforts at other institutions performed within the past year.

- Joshua Fu at the University of Tennessee is working towards using SMOKE for China and Taiwan. This effort has been funded by the US EPA and includes updates to files and code needed to handle different time zones, region names, and diurnal patterns.
- Environment Canada, Alberta Environment, and the Clean Air Strategic Alliance (CASA) are using SMOKE to prepare emissions from western Canada and the northwestern US for input to CMAQ. (Dave Fox [dave.fox@ec.gc.ca])
- The Northwest Regional Modeling Center (NWRMC) applied SMOKE, MM5, and CMAQ to model ozone and aerosols over a two-week period in July 1996. The domain of 12-km grid cells included the 3-state region (ID, OR, and WA) and southern British Columbia. Major participants in the project included the Idaho Department of Environmental Quality, Oregon Department of Environmental Quality, Washington State Department of Ecology, EPA Region 10, Washington State University, and Environment Canada. (Sally Otterson [sott461@ecy.wa.gov])
- The Illinois State Water Survey has used SMOKE with the 1996 National Emission Inventory and also projected 2020 emissions to produce a 3-month air quality simulation over the U.S. at 90-km resolution and the Midwest at 10-km resolution. Contact: (Allen Williams [allenwil@uiuc.edu])

7 RELEASE AND SUPPORT ISSUES

One of the primary challenges for the community in using SMOKE is the erratic timing of releases and bug fixes, and the overall quality of the testing and contents of those releases. To date, MCNC has supported most of the cost of preparing and testing SMOKE releases, but this has resulted in less-than-optimal time spent on testing and debugging. We are currently seeking community funding for correcting SMOKE bugs in a timely manner, creating appropriate test cases, providing frequent and high-quality releases of the SMOKE software, and maintaining a SMOKE release website. I estimate that the total cost of these activities on an annual basis is about $35K. This cost could easily be shared among the many SMOKE user organizations to better provide SMOKE to that community. This would result in higher quality releases that would save time, money, and aggravation for all users.

8 CONCLUSIONS

The past year or so has been quite active for the SMOKE modeling system and I look forward to continued new challenges and applications for it. Although the continued rapid development of SMOKE will surely make this document out of date soon, I have attempted to provide a snapshot of SMOKE that is intended to quickly inform readers of SMOKE's status.

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