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Implementing the SMOKE Emissions Processing System with WRF-Chem: Progress and Early Results

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1. INTRODUCTION

Work on the chemistry version of the Weather Research and Forecasting Model (WRF-Chem) is progressing (Grell et al., 2003). The current development version features online coupling between the meteorology and chemistry to account for the integrated effects of both. To date, however, emissions estimates—with the notable exception of biogenic emissions—have been provided to the model using historical data not linked to the integrated model solution. This does not account for the meteorologically dependent portions of point, area, and mobile emissions sources, which will be important as the model progresses towards operational status. Further, it does not interact with geo-spatial emissions data that natively resides either at points or within/along irregularly shaped regions such as counties or roads.

In this paper, the implementation of an online emissions modeling approach, using the Sparse-Matrix Kernel Emissions Processing System (SMOKE; Coats, 1996; Houyoux et al., 2000), will be described. SMOKE is being used as the emissions processing/modeling system of choice in a number of present-day air quality modeling systems (McHenry et al., 2003), and is considered the state-of-the-art currently available. SMOKE is in actuality a series of programs that process foundational emissions inventory data while speciating the inventory and performing selected pre-calculations in preparation for input into a3D atmospheric chemistry model.

A functional design of a typical SMOKE implementation, depicting processing for a single inventory, is shown in Figure 1. Here, meteorological data is input into three of five processing steps, including mobile, biogenic, and point source plume rise, to arrive at a merge and transform intermediate step. The meteorology that is initially input is interpolated from gridded-model-space to the pertinent geo-spatial coordinate of the emissions category being modeled. Then, at the merge-transform step, the combined effects of each source for every relevant species, e.g. NO, NO_2, etc., are aggregated to the grid accounting for only those line segments and point sources that lie within each grid cell.

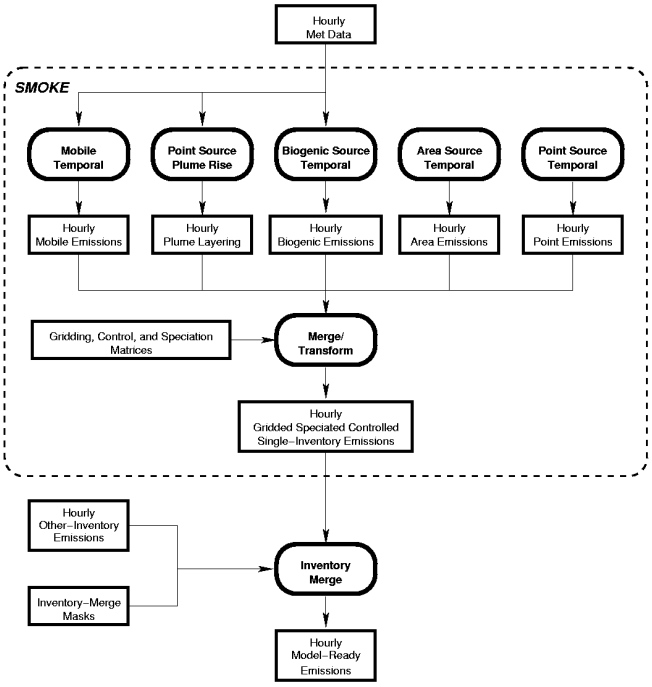

Figure 1. *Typical SMOKE implementation within an operational air quality forecasting system.*

The results of the merge-transform step, during which a control or perturbation matrix may also be applied, are time-stepped, gridded, speciated emissions for that inventory being processed. Below and to the left of the dotted box, Figure 1 shows two additional boxes which provide for separate instantiations of different inventories that may be used in combination (defined by "merge-masks") with the primary instantiation shown within the

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dotted box. Each additional inventory could be as complex as the primary inventory, or, could incorporate only certain emissions categories. This feature is particularly important for operational forecast modeling because it allows the operational "inventory" to evolve and improve over time as new data becomes available through local, state, regional, or international inventory developers.

2. WRF-SMOKE SYSTEM DESIGN

The design of the SMOKE implementation within the WRF-Chemistry system accounts for both the accurate geo-spatial modeling and the multiple-inventory-merge capability described above. In order to accomplish this, SMOKE is being implemented within the WRF-Chem system as a cooperating peer-to-peer model, rather than as an embedded submodel. Thus, WRF-Chem writes meteorological data to a "file," which may either be stored on-disk or in memory, and then each of the relevant SMOKE emissions-category-processors reads the data and performs relevant calculations before the merge steps write the data back out for WRF-Chem to read for the next time-step. In WRF-Chem, emissions are processed at the end of each meteorological internal time-step.

A highly simplified example is shown schematically in Figure 2, where three different geo-spatially defined emissions inventories are each needed for a single simulation. Here, three separate copies of SMOKE must be run in order to process the data and provide for meteorological interactions, prior to the final merge step. Because of SMOKE's computational efficiency, this represents a negligible fraction of the overall simulation wall-clock time, while providing for the ability to process and merge many different inventories within a single simulation.

Implicit in this example is the accurate geo-spatial modeling already noted. This allows the crucial effects of meteorology on all relevant emissions source categories to be accurately accounted for at every model time step. Currently, this includes all categories except "area" sources, though it can be argued that this category should be included in the future.

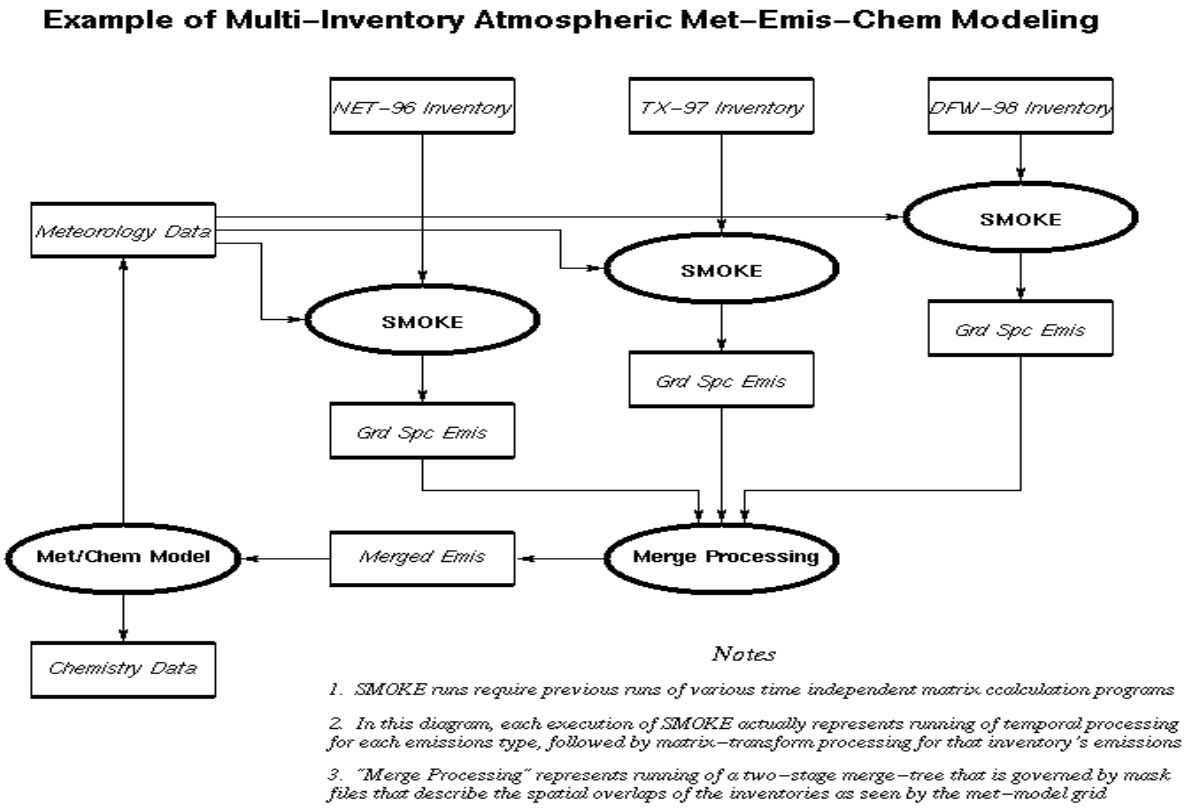

Figure 2. *High-level dataflow diagram depicting SMOKE as a peer-to-peer, rather than embedded, model within a coupled met-chem-emissions simulation.*

To properly model this, the following meteorological variables are passed into SMOKE:

- **Temperature**, used in mobile and biogenic emissions, and point source plume rise.
- **Pressure**, used in point source plume rise.
- **Humidity**, used in biogenic emissions.
- **Atmospheric stability**, used in point source plume rise.
- **Wind speed**, used in biogenic emissions, and point source plume rise.
- **Photosynthetically-active radiation**, used in biogenic emissions.

Modifications to the currently "released" version of SMOKE, maintained at the "Community Modeling and Analysis Systems (CMAS)" Web-site (http://www.cmascenter.org) by the Carolina Environmental Program at the University of North Carolina (http://www.cep.unc.edu/empd/index.shtml) at Chapel Hill, are also required by the present implementation. Several reasons necessitate these modifications. First, the current release (unlike earlier releases) violates the object/class analysis for "time-stepped model program" that was initially an inherent part of the system design (Coats, 1995). In the current release, a "pollutant groups" feature was added under which all of the time-steps for one subset of pollutants are processed before the start of processing for other pollutant groups.

Second, the currently released version is structured such that it may override the user's run configuration (e.g. for the time-period being modeled) *and actually perform some other set of emissions modeling than was specified*, while reporting "normal successful completion" in the meantime. In addition, ***INCLUDE*** and ***MODULE*** dependencies are being removed to restore maintainability—since the current structure tends to hide these dependencies. Further, "private," potentially obsolete copies of external libraries are being revised for compatibility with public I/O API routines(http://www.baronams.com/products/ioapi) (Coats et al., 1995) that will form the basis for data-exchange between the WRF-Chem model and the SMOKE system. Finally, private copies of I/O API subroutines, constants, and data structures are being removed.

SMOKE enhancements, beyond the current release, are also under development to support peer-to-peer model data exchange:

(1) SMOKE is being revised to handle time-steps other than the currently hard-coded hourly time-step for input meteorology data. Time-steps will be allowed that exactly divide the one-hour time step of SMOKE's temporal profile tables.

(2) Relevant SMOKE sub-models are being parallelized. It is unrealistic to expect a single-processor implementation of SMOKE to efficiently cooperate with a WRF-Chem that may be running on hundreds of processors.

(3) SMOKE is being re-coded so that proper attention is paid to failure-status returns for library calls that evaluate I/O status, environment-variables, etc.

(4) The SMOKE build (make) system is being restructured so that it is compatible with the above mentioned I/O API build system, which itself has been restructured, in Version 2.2, for compatibility with the WRF build system. Two concerns are referential integrity and link-compatibility, both of which are already known to be problems with SMOKE.

3. SYSTEM TESTING

The system is currently in the early stages of testing in a hybrid SMP/MPP environment. Examples of early results from these tests will be shown at the conference.

4. CONCLUSIONS

Work on the WRF-Chemistry model is progressing and includes implementation of an advanced emissions modeling system allowing for much better geo-spatial representation of the effects of meteorology on emissions while implementing the capability to merge several different inventories within a single simulation-execution. This feature will be crucial for real-time operational forecasts for which accuracy in the emissions component of the modeling system is a first-order requirement.

It can be envisioned that for real-time forecasting, the WRF-CHEM emissions system will need to ingest *event-driven emissions* (from sources such as forest fires or accidental chemical releases) and *observed episode specific emissions.* Event driven emissions either require observational data (e.g., from satellites), sufficient foundation files for first-principles modeling of forest fires (etc.), or both. Episode specific emissions are observed time stepped emissions values for specific sources; typically, they are available only in retrospective studies. SMOKE, for example, has a "substitution step" in which these emissions can be added or substituted into the modeled source level time stepped emissions, so that inclusion of this kind of data is *not difficult, once it is available*.

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REFERENCES

Coats, C.J., Jr., A.F. Hanna, D. Hwang, and D.W.Byun, 1995: Model engineering concepts for air quality models in an integrated modeling system. In *Regional Photochemical Measurement and Modeling Studies, Transactions*, J.G. Watson, J. C. Chow, and P.A.Solomon, Eds., Air and Waste Management Association, San Diego, CA

Coats, C.J. Jr., 1996: High-performance algorithms in the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. *Proc. Ninth AMS Joint Conference on Applications of Air Pollution Meteorology with A&WMA*, Amer. Meteor. Soc., Atlanta, GA, 584-588.

Davidson, Paula, 2003: National air quality forecast capability: first steps toward implementation. *Program Overview, National Air Quality Forecast Capability,* NWS, Office of Sci/Technology, http://www.nws.noaa.gov/ost/air_quality

Grell, G. A., S. Emeis, W. R. Stockwell, T. Schoenemeyer, R. Forkel, J. Michalakes, R. Knoche, W. Seidl, 2000: Application of a multiscale, coupled MM5/chemistry model to the complex terrain of the VOTALP valley campaign. *Atmospheric Environment* **34** 1435-1453.

Grell, G. A., S. E. Peckham, R. Schmitz, and S. A. McKeen, 2003: Fully coupled "online" chemistry within the wrf model: a description and some applications. Paper 12.6, *Proc. 20th Conference on Weather Analysis and Forecasting/16th Conference on Numerical Weather Prediction,* Amer. Meteor. Soc., Seattle, Wash.

Houyoux, M.R., J.M. Vukovich, C.J. Coats, Jr., N.W. Wheeler, and P.S. Kasibhatla, 2000: Emission inventory development and processing for the seasonal model for regional air quality (SMRAQ) project. *J.. Geophys. Res.*, *Atmospheres*, **105**(D7), 9079-9090.

McHenry, J.N., D. Byun, C. Coats ,Adel Hanna, R. Mathur, K. Schere, U. Shankar, J. Olaguer, A. Xiu, 2001: Design considerations for the WRF-Chemistry model: a white paper. Available from the author, *Baron Advanced Meteorological Systems, PO Box 110064, RTP, NC, 27709-5064*; Email: john.mchenry@baronams.com .

McHenry, J.N., W.F. Ryan, N.L. Seaman, C.J. Coats Jr., J. Pudykeiwicz, S. Arunachalam, and J.M. Vukovich, 2003: A real-time eulerian photochemical model forecast system: overview and initial ozone forecast performance in the NE US corridor. Accepted for publication, *Bull. Amer. Meteor. Soc.*

Peckham, S., G.A. Grell, and S. McKeen, 2003: Comparisons between observations made during neaqs and air quality forecasts from MM5 and WRF chemistry models. Paper J2.15, *Proc. Sixth Conference on Atmospheric Chemistry: Air Quality in Megacities,* Amer. Meteor. Soc., Seattle, Wash.