

# REAL-TIME NESTED MESOSCALE FORECASTS OF LOWER TROPOSPHERIC OZONE USING A HIGHLY OPTIMIZED COUPLED MODEL NUMERICAL PREDICTION SYSTEM\*\*

John N. McHenry<sup>1\*</sup>, Nelson Seaman<sup>2</sup>, Carlie Coats<sup>1</sup>, Annette Lario-Gibbs<sup>2</sup>, Jeff Vukovich<sup>1</sup>,  
Neil Wheeler<sup>1</sup>, Dave Stauffer<sup>2</sup>, Elizabeth Hayes<sup>3</sup>

<sup>1</sup>Environmental Programs  
MCNC–North Carolina Supercomputing Center  
Research Triangle Park, North Carolina

<sup>2</sup>Department of Meteorology, The Pennsylvania State  
University, University Park,  
Pennsylvania

<sup>3</sup>Silicon Graphics Inc.  
Environmental Sciences Group  
MCNC-North Carolina Supercomputing Center, Research Triangle Park, North Carolina

\*\* This paper appears in substantially the same form in *Preprints: Symposium on Interdisciplinary Issues in Atmospheric Chemistry, Jan 1999, Dallas, Tx. American Meteorological Society*

## 1. INTRODUCTION\*

Recently, “third generation” air quality modeling systems such as MCNC’s Multiscale Air Quality Simulation Platform (MAQSIP) and EPA’s Models-3/CMAQ (Community Multiscale Air Quality) model have been developed to address multiscale, multipollutant problems. In the case of MAQSIP, atmospheric scientists and chemists have worked closely together with computational scientists and mathematicians to create a modular, flexible modeling system.

In the U.S., the paradigm for using such systems has been to apply them in retrospective historical simulations in order to contribute to policy assessments and engender additional scientific progress. However, the progress that can be made using such a paradigm is ultimately constrained by a limited number of test cases that are chosen for resimulation, evaluation, aggregation, and analysis. Unlike numerical weather prediction, which by its very nature involves multiple runs of multiple models at multiple centers every day of the year, air quality modeling has not been able to benefit from the wide application and scientific advancements that result from repeated forecast applications of the available state-of-science models.

Now, through the close coupling of MAQSIP, the Sparse Matrix Operator Kernel for Emissions (SMOKE, Coats, 1996), and the PSU/NCAR MM5 Mesoscale Model (Grell et al., 1994), the ability to make timely, quasi-operational real-time atmospheric chemical forecasts using state-of-science models has been demonstrated. During the summer of 1998, this

tripartite coupled model was used to produce once-daily, experimental, real-time 48-hour numerical air quality predictions (NAQPs) on a nested 108-36km grid covering the CONUS (MCNC, 1998; Penn. State, 1998).

The forecasts were produced on a 4-processor Silicon Graphics, Inc., Power Challenge computer at the Penn. State University Dept. of Meteorology, and involved close cooperation between atmospheric and computer scientists at MCNC-North Carolina Supercomputing Center, Penn. State, and SGI.

## 2. COMPONENT MODELS

MM5 has been run in real-time at Penn State for nearly a decade (Warner and Seaman, 1990). It has gone through significant development since that time including the transition from a hydrostatic to a fully compressible non-hydrostatic model. Initial and boundary conditions are supplied through UNIDATA (UCAR, 1998), and drawn from the 32km ETA forecasts aggregated to GRID 104. MM5’s coarse (108km) domain covers most of North America from the arctic circle south to Panama, and includes large portions of the eastern Pacific and western Atlantic. The fine 36km domain covers the CONUS. Both MM5 domains use a Lambert conformal map projection with 30 sigma-coordinate layers in the vertical. Model top is fixed at 100mb. The MAQSIP domains (Figure 1.) are windows into these MM5 domains and share this common vertical structure.

MM5 is configured with a 1.5 order TKE boundary layer scheme (Gayno, 1994), a deep convection scheme (Kain and Fritsch, 1993), a simple ice phase explicit moisture scheme, an atmospheric radiation scheme (Dudhia, 1989), and its standard land-surface model. A shallow convection scheme is being developed under another project and will be added later (Deng et al., 1998); it is designed specifically to support the needs of air quality models.

---

\*Corresponding author address: John McHenry, MCNC, P.O. Box 12889, 3021 Cornwallis Rd., Research Triangle Park, NC, 27709; E-mail: mchenry@mcnc.org

MAQSIP is a modular modeling system which, for this application, is configured for prediction of lower tropospheric ozone. This configuration uses a modified version of the Carbon Bond IV (Gery et al., 1989) chemical mechanism, a flux-form advection scheme (Bott, 1989), a K-theory scheme for turbulent vertical re-distribution of pollutants (Alapaty et al., 1997), and a dry deposition scheme (Walcek, et al., 1986). Clear-sky photolysis rates are calculated



**Figure 1. MAQSIP Real-time Domains: Coarse Domain-108km; Fine (Nested) Domain--36km**

following Madronich (1987). It also uses a brand new cloud processes package which represents the effects of deep and shallow convection, stratiform layer clouds, and additional sub-grid clouds.

The cloud package accounts for sub-grid vertical redistribution of pollutants, pertinent aqueous chemical reactions, scavenging/wet deposition, and cloud-attenuation of actinic flux. It is particularly closely coupled to MM5's deep convective and resolved scale moisture parameterizations, making use of a 1:1 link between the Kain-Fritsch parameterization in MM5 and a chemical counterpart to that scheme in MAQSIP. Prototypes have been previously reported (McHenry et al., 1996; McHenry and Binkowski, 1996), and more details will be forthcoming.

The turbulence parameterization utilizes predicted boundary layer heights from MM5 to limit vertical mixing. Closer coupling via direct ingestion of eddy diffusivities is planned for the very near future.

SMOKE is a high-efficiency emissions processing system. It features several hundred-fold computational performance enhancements due to its sparse-matrix algorithms for factor-based computations. It consumes less than 10 minutes of execution time on MAQSIP's 108-36km nested grid. The real-time simulations use SMOKE to process an improved Ozone Transport

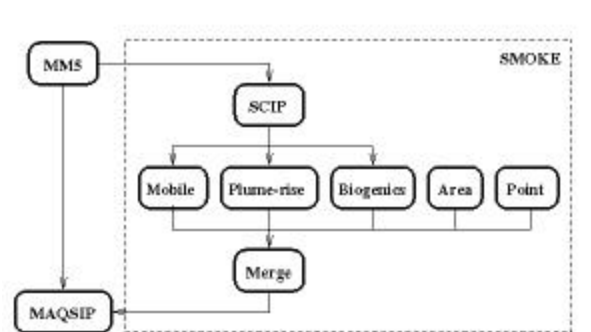
Assessment Group (OTAG) 1995 emissions inventory (Pechan, 1996), the same inventory used in a historical MAQSIP ozone simulation of the summer-season of 1995. Those historical results will be reported elsewhere. For this real-time application, no attempt was made to project the inventory to 1998, but an emissions projection model could be easily added.

For the first time, real-time *forecast* meteorology was fed from MM5 to SMOKE to model meteorologically sensitive phenomena such as biogenic and vehicular emissions, and point-source plume rise. Because of the higher vertical resolution in third-generation models, SMOKE's discretization of plume rise *for every point source* was appropriately used.

### 3. MODEL COUPLING AND FORECAST EXAMPLE

Figure 2 shows the high-level dataflow diagram for the real-time system. An output module, MCPL (Coats et al., 1998), was developed within MM5 to generate outputs compatible with SMOKE and MAQSIP, which both use an I/O Applications Programming Interface (I/O API, Coats, 1995). The present I/O API implementation is layered on top of netCDF (Rew 1990), from the National Center for Atmospheric Research, although the I/O API was designed from the beginning so that this lower layer could be easily changed.

MCPL fits into MM5 with minimal effort, and is callable at a variety of time scales from the advection-step frequency on up. It provides functionality generalizing the present MM5 subroutine OUTTAP. It is extremely flexible and configurable, allowing selected output variables, output formats, and windows into MM5 nests, all through the use of environment variable flags. For this application, MCPL is called every simulation hour for both the coarse and fine MAQSIP domains.



**Figure 2. MM5-SMOKE-MAQSIP Model-Coupling**

As Figure 2. indicates, MM5 (top left) is first run on both its coarse (108km) and fine (36km) domains.

Then, a small interface processor (SCIP) is used to build a database of Kain-Fritsch deep convection soundings for use in MAQSIP. SCIP also constructs cloud fractional coverage and liquid water contents using algorithms in MAQSIP's new cloud package. This provides SMOKE with the self-consistent cloud data needed to account for attenuation of the photosynthetically active radiation (PAR) that drives biogenic emissions. Once SMOKE finishes, all data is prepared and MAQSIP is ready to run, first on the coarse domain, then on the fine domain.

MAQSIP was extensively re-written to run efficiently on microprocessor-based parallel machines. Algorithm logic was refactored to provide stride-1 memory access and longer basic blocks yielding reduced memory traffic, better register re-use and cache coherency, and larger parallel work tasks. Subroutines were restructured for parallel callability, and OpenMP and SGI PFA parallel directives were inserted. Many other general optimizations were performed as well. Run-times on the target machine were reduced from approximately 14 hours on a single CPU to under 3 hours on 4 CPUs. Typically, the 48 hour MAQSIP forecast is now completed by 8AM EDT—barring Unidata problems—in time to provide numerical guidance for this afternoon's and tomorrow afternoon's ozone outlook.

There is little real-time atmospheric chemical measurement data. Ground level ozone data are just beginning to be collected and reported east of the Mississippi. There is no regular ground level primary precursor data ( $\text{NO}_x$ , VOC) or are there regular upper air chemical sounding data. Thus, establishing initial and boundary conditions for MAQSIP is more problematic than for meteorological models. For boundary conditions, clean tropospheric background concentrations are set on the boundaries of the coarse domain, including a climatological vertical ozone profile as a function of latitude. The fine domain utilizes time-dependent chemical boundary conditions provided by the coarse domain MAQSIP run. Within the coarse domain, the emissions database extends to just east of the Rockies allowing for adequate build-up of polluted air upwind of the fine domain boundary.

Initial conditions for both domains are determined, at present, by using the 24 hour forecast concentrations from the previous day's forecast; or, in the case when the model needs to be restarted, from a "cold start" file. We will implement somewhat better techniques shortly, but, without daily or twice-daily atmospheric chemical measurements, the establishment of initial conditions will remain one of our largest sources of forecast uncertainty.

Figure 3. shows an example forecast of peak 1-hour surface layer ozone for Aug 28, 1998. The peak 1-hour concentrations were determined by extracting the hourly forecasts and selecting the peak hourly value at each cell, consistent with the traditional exceedence metric. The forecast was initialized at 00UTC the same day. Peak hourly values range up to 125 PPB at cell (22,17), and other maxima, in the 100-124 PPB range, are indicated in a narrow corridor paralleling the Ohio River along the Ohio-West Virginia border. Broad minima are apparent over New Jersey, Delaware and southeast Maryland.

By comparison, Figure 4. shows the observed surface level ozone collected from an array of local and state ozone monitors and assembled for display on the EPA's "AIRNOW" Web-site (EPA-OAQPS, 1998). States which do not yet report data are very dark grey, and all water bodies are shown in black. MAQSIP performs quite well in capturing the broad mesoscale peak ozone features. The line demarking the transition from below to above 60 PPB is well-represented, extending from central Illinois east-northeast across southern New England in both the observations and forecast. In the Ohio Valley, peak hourly values above 80 PPB are also captured reasonably well. MAQSIP predicts an area of such peaks in the southern half of Illinois, whereas the observations show this area shifted to the east in southern Indiana. MAQSIP shows a small peak above 100 PPB in west central Kentucky, consistent with the observations. Because West Virginia didn't report any data, the smoothing algorithm used to display the observations near the Ohio-WV border may not quite capture the actual peak magnitudes displayed there, which are about 10 PPB less than the MAQSIP prediction. Observed 80-100 PPB peaks in southern Pennsylvania, portions of southwest Virginia and the western Piedmont of North Carolina are underforecast by MAQSIP, but MAQSIP represents the clean air over New Jersey and the DelMarva peninsula exceptionally well.

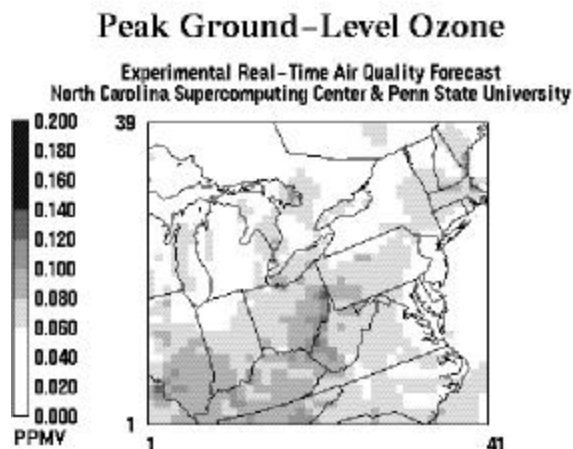


Figure 3. MAQSIP Forecast Peak Hourly Ground Level Ozone, Aug. 28, 1998, 36km domain.

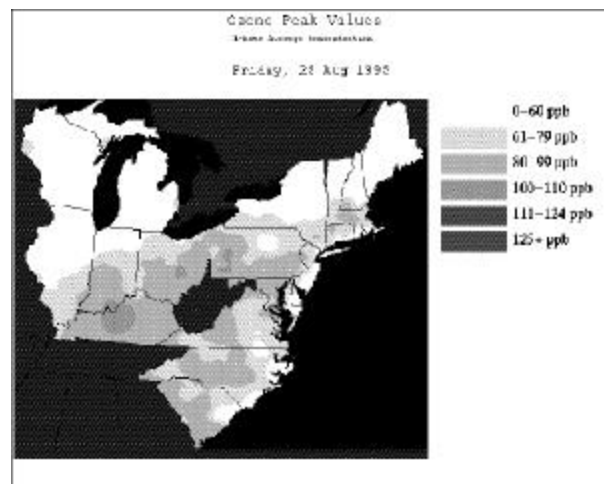


Figure 4. Observed Ground Level Peak 1-Hour Average Ozone Values, Aug. 28, 1998.

#### 4. CONCLUSIONS

For the first time in the U.S., a quasi-operational state-of-science atmospheric chemistry prediction model has been deployed. We have demonstrated that it is possible to complete a 48-hour forecast in a timely manner, such that numerical air quality guidance could be provided to state and local officials interested in issuing air quality alerts. A simple forecast example was used to show the potential that the coupled model has measurable skill. More in depth results will be reported elsewhere.

The cross-fertilization between operational modeling and basic research has proven its value within the pure atmospheric sciences. We believe that the time to use this approach within the atmospheric chemical community has now arrived.

*Disclaimer.* Although the research described in this article has been funded wholly or in part by the United States Environmental Protection Agency through Grants #R825210 and #R825211 to MCNC and Grant #R825254 to Penn State University, it has not been subjected to the Agency's required peer review and policy review and therefore does not necessarily reflect the views of the Agency and no official endorsement should be inferred. Mention of trade names/products does not imply official endorsement.

#### REFERENCES

- Alapaty, K., J.E. Pleim, S. Raman, D.S. Niyogi, and D.W. Byun, 1997: Simulation of atmospheric boundary layer processes using local- and nonlocal-closure schemes. *J. App. Met.* **36**,3,214-233.
- Bott, A., 1989: A positive definite advection scheme obtained by nonlinear renormalization of the advective fluxes. *Mon. Wea. Rev.*, **117**, 1006-1015.
- Coats, C.J., 1995: The EDSS/Models-3 I/O applications programming interface. <http://envpro.ncsc.org/products/iaoapi/index.html> MCNC Env. Programs, RTP NC.
- Coats, C.J., 1996: High performance algorithms in the sparse matrix operator kernel emissions (SMOKE) modeling system. *Ninth AMS Joint Conference on Applications of Air Pollution Meteorology with A&WMA*. Amer. Meteor. Soc., Atlanta, 584-588.
- Coats, C.J., J.N.McHenry, A. Lario-Gibbs, and C.D.Peters-Lidard, 1998: MCPL(): A drop-in MM5-V2 module suitable for coupling MM5 to parallel environmental models; with lessons learned for the design of the weather research and forecasting (WRF) model. *The Eighth PSU/NCAR Mesoscale Model Users' Workshop*. MMM Division, NCAR, Boulder, Co., 117-120.
- Deng, A., N.L.Seaman, and J.S.Kain, 1998: A parameterization for detraining cumulus-cloud mass into dissipating layer clouds. *Twelfth Conference on Numerical Weather Prediction*. Amer. Meteor. Soc., Dallas, 120-123.
- Dudhia, J., 1989: Numerical study of convection observed during the winter monsoon experiment using a mesoscale two-dimensional model. *J. Atmos. Sci.*, **46**, 3077-3107.
- EPA-Office of Air Quality Planning and Standards (OAQPS), 1998: Ozone mapping project, environmental monitoring for public access and community tracking. <http://www.epa.gov/airnow/>

- Gayno, G.A., 1994: Development of a higher order, fog producing boundary layer model suitable for use in numerical weather prediction. M.S. Thesis. Dept. of Meteorology, Penn State University.
- Gery M.W., G.Z. Whitten, J.P. Killus, and M.C. Dodge, 1989: A photochemical kinetics mechanism for urban and regional scale computer modeling. *J. Geophys. Res.*, **94**, 12925-12956.
- Grell, G.A., J. Dudhia, and D.R. Stauffer, 1994: A description of the fifth-generation Penn State/NCAR mesoscale model (MM5). NCAR Technical Note TN-398, Bldr. Co.
- Kain, J.S., and J.M. Fritsch, 1993: Convective parameterization for mesoscale models: the Kain-Fritsch Scheme. *Meteor. Mono.* **24**, No. 46, Amer. Meteor. Soc., Boston.
- MCNC, 1998: Numerical air quality prediction (NAQP) web-site. <http://envpro.ncsc.org/NAQP>
- Madronich, S., 1987: Photodissociation in the atmosphere. 1. Actinic flux and the effects of ground reflections and clouds. *Jou. Geophys. Res.* **92**, D8, 9740-9752.
- McHenry, J.N., J.S. Kain, and J. Pleim, 1996: Development and testing of a Kain-Fritsch based deep convective cloud chemistry scheme for incorporation into multiscale air quality models. *Ninth J. Conference on Air Pollution Meteorology with the Air and Waste Management Association*. Amer. Meteor. Soc., Atlanta, 207-212.
- McHenry, J.N., and F.S. Binkowski, 1996: Development and testing of a Betts-Miller based shallow convective cloud chemistry scheme for incorporation into multiscale air quality models. *Ninth J. Conference on Air Pollution Meteorology with the Air and Waste Management Association*. Amer. Meteor. Soc., Atlanta, 254-259.
- Pechan, E.H., and Assoc., 1996: Ozone transport assessment group emissions inventory development report, volume II, version 1.0. *Pechan Report No. 68-D3-0035*, Durham, NC.
- Penn. State, 1998: NAQP web-site: <http://mm5.met.psu.edu/mm5/MM5maps.html>
- Rew, R.K., G.P. Davis, 1990: "NetCDF: an interface for scientific data access." *IEEE Computer Graphics and Applications* **10**: 76-82.
- UCAR UNIDATA, 1998: Unidata Internet Home Page. <http://www.unidata.ucar.edu/>
- Walcek, C.J., R.A. Brost, J.S. Chang, and M.L. Wesely. 1986. SO<sub>2</sub>, sulfate, and HNO<sub>3</sub> deposition velocities computed using regional land-use and meteorological data. *Atmos. Environ.* **20**:949-964.
- Warner, T.T., and N.L. Seaman, 1990: A real-time weather-prediction system used for research, teaching, and public service at the Pennsylvania State University. *Bull. Amer. Meteor. Soc.* **71**, 6, 792-805.