2.15 Toward a US National Air Quality Forecast Capability: Current and Planned Capabilities

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Abstract In partnership with the US Environmental Protection Agency (EPA), the National Oceanic and Atmospheric Administration (NOAA) has deployed the initial stages of a national air quality forecast capability into the National Weather Service operational suite. Current capabilities provide next-day, hour-by-hour, 12-km resolution predictions of (1) ground-level ozone (O_3) for the Eastern U.S. and (2) smoke for the lower 48 states. These are generated twice daily by NOAA's National Centers for Environmental Prediction with linked weather and air quality models: the NOAA-EPA Community Multiscale Air Quality model driven by NOAA's operational North American mesoscale weather prediction model. Forecast accuracy is verified with O_3 observations compiled by EPA and with satellite-derived smoke observations. Future operational capabilities for nationwide O_3 forecasts are targetted within three years, to be followed by quantitative particulate matter forecasts, and extended forecast periods. Expansion will proceed as rapidly as resources and achievement of required test accuracy permit.

Keywords Air quality forecasts, O_3 forecasts, smoke forecasts, $PM_{2.5}$ prediction

1. Introduction

As mandated by Congress, NOAA is establishing a US national air quality (AQ) forecast capability. This capability is being built in partnership with EPA, to provide AQ forecast information with enough accuracy and lead-time so that people can take actions to limit harmful effects of poor AQ.

NOAA and EPA researchers recently celebrated 50 years of collaboration in AQ research. As a result of this collaboration and related research in atmospheric chemistry modeling, techniques to simulate atmospheric chemical transport driven by numerical weather models had progressed to the extent that by the mid-1990s, NOAA and EPA had built a retrospective modeling capability, the Community Multiscale Air Quality (CMAQ) model (Byun and Schere, 2006) appropriate for state and local agencies' EPA-required analyses of factors affecting air pollution. Several countries, e.g. Canada and Australia, began experimenting with real-time numerical AQ predictions, based on similar photochemical models to predict ground-level O_3 (CHRONOS; Pudykiewicz et al., 1997) and/or Lagrangian transport

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models (HYSPLIT; Draxler and Hess, 1998). In the US, constituents from the public and private sectors urged NOAA to begin providing AQ predictions operationally. Then Congress acted: the Senate passed an amendment to the Energy Policy Act of 2002 which directed NOAA to begin producing operational AQ forecast guidance, for which Congress began directing appropriations to NOAA. NOAA undertook to build this capability in partnership with EPA, to leverage the respective strengths of the two agencies in atmospheric prediction and air pollution science, as formalized in a Memorandum of Agreement for AQ forecasting activeties signed in 2003 by the EPA Administrator and the Deputy Director of the Department of Commerce (NOAA's parent organization).

The initial operational capability, deployed in September 2004, provided next-day O_3 predictions for a Northeast US domain. Additional development and testing succeeded in extending the operational forecast domain to the entire Eastern US (August 2005) and the contiguous 48 states (CONUS) (September 2007). The guidance products (example in Figure 1) provide hour-by-hour predicted ground-level O_3 concentrations, at 12 km grid resolution. Predicted O_3 concentrations are shown on NOAA dataservers and represented by the health-based AQ Index on EPA's AIRNow dataserver. In March 2007, an initial operational capability for smoke predictions over the CONUS was implemented. The smoke predictions, at12km resolution, updated once daily, simulate transport of smoke (O'Neill et al., 2007) from fires detected by satellite. Ongoing development efforts are aimed at expanding the capability to nationwide O_3 and smoke coverage within three years, and to begin providing particulate matter (PM) forecasts within five years.

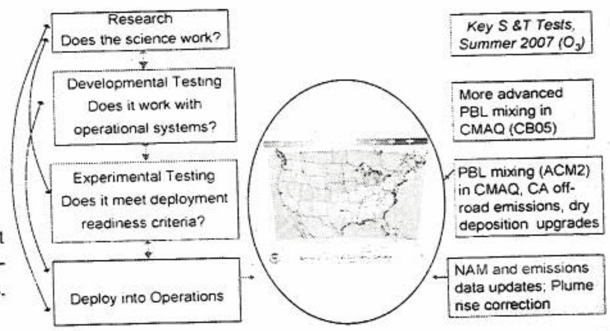

Fig. 1 Development and test phases to prepare for deployment into NWS operations. Summer 2005

Via phased development, testing, and implementation, the operational AQ forecast capability is being upgraded with advanced science, algorithms, and simulation techniques, in testing with expanded domains and additional forecasted elements. Figure 1 illustrates generalized transition phases employed by the NWS to move research capabilities into operations, along with specific tests during 2005 that led to the first expansion of the initial operational capability. To ensure required operational product accuracy and reliability, specific operational readiness benchmarks must be demonstrated within objective verification, subjective feedback, and engineering readiness categories. Some of the summer 2005 test improvements (e.g. better treatment of large-scale convective processes) to the AQ forecast system were needed merely to maintain required forecast accuracy over larger domains – contrary to expectation, initial developmental testing over expanded domains did not improve prediction accuracy (Lee et al., 2008). A number of other 2005 and 2006 test improvements (e.g. use of radiation fields simulated in the weather model to modify photolysis rates) are helping to increase coupling between the CMAQ and Eta's replacement model, the WRF-NMM.

Developmental testing is also underway for components needed to establish a PM forecast capability. A CMAQ-aeroaol option that NWS is testing, like other systems currently in use (WRF-Chem; Grell et al., 2005; BAMS; McHenry et al., 2004; CHRONOS, Pudykiewicz et al., 1997; AURAMS, Gong et al., 2003), is based on inventories of primary emissions sources and secondary aerosol formation in the atmosphere. While the NOAA aerosol test-prediction accuracy lags far behind the O_3 predictions, the NAM/CMAQ-aerosols results compared favourably with other models tested with the 2004 ICARTT campaign (McKeen et al., 2007).

Near-term goals of phased development and testing are to expand the operational capabilities to nationwide coverage and add PM predictions; longer-term goals include extending the forecast range and adding other significant pollutants to the forecasted elements.

2. Current Operational Capability

Figure 2 illustrates the end-to-end AQ forecast capability (Davidson et al., 2004 and 2007). NCEP's North Americal Mesoscale weather forecast model (NAM) is operationally linked to CMAQ, developed by NOAA researchers at EPA originally for AQ regulatory analysis. Adaptations and interfaces built to drive CMAQ in real-time predictions with the NAM, then Eta-12, but as of June, 2006, WRF-NMM, are described by Otte et al. (2005). Dynamic weather observations are assimilated four times daily into the NAM. Pollutant emissions data are derived from the EPA's National Emissions Inventory. The module PREMAQ preprocesses emissions, to incorporate weather dependence, for the reactive chemical transport simulations of CMAQ, producing O_3 concentration predictions.

Hourly predictions at 12km resolution, through midnight next day, are provided on operational NOAA and EPA dataservers; examples are shown within Figure 2. Ground-level O3 concentrations are provided as both 1-hour and 8-hour averages, and updated twice daily. Ground-level smoke concentrations, along with column-averages, as 1-hour averages, are updated once daily. NOAA's operational products are available on www.weather.gov/aq in time for AQ forecasters to use in issuing their next-day AQ alerts, and for people at risk to use in planning daily activities to minimize their exposure to poor AQ. On EPA's AIRNow site, the O_3 predictions are shown as health-based AQ Index categories. State/local AQ forecasters issue AQ alerts for some 300 cities across the US based on expected elevated O_3 concentrations; for 100 of those cities, they also consider expected PM. Feedback links are provided for collecting user comments. NOAA and EPA also work actively with state and local AQ forecasters who participate in a focus group for developmental test products. The focus group forecasters share their expertise and feedback with our development team, improving product utility and reliability.

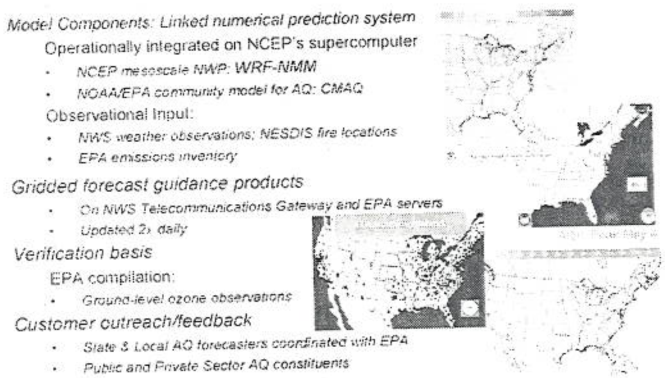

Fig. 2 End-to-end air quality forecast capability

3. Improving the Current Capability

In order to reach goals of nationwide coverage for O_3 and PM predictions with sufficient accuracy and timeliness, a number of challenges need to be overcome: 1) computational efficiency, 2) maintaining accuracy over expanding domains with increasingly diverse pollution sources, weather patterns and domains, 3) adding important sources of airborne PM not included in emissions inventories, and 4) improving quantitative predictions of PM formation, transformation, transport and deposition. NOAA's progress toward addressing these issues is outlined below.

With the current operational configuration, sequential predictions of weather (NAM) followed by AQ (CMAQ), the AQ forecast model run-time window is two hours. The requirement ensures product availability for AQ forecasters based on the most current weather predictions, and takes into account the 30 minutes needed for interface processing between NAM and CMAQ, product post-processing, communications and display generation. NWS' operational weather and climate supercomputing facility has been augmented to include AQ prediction requirements.

To meet the operational run-time requirement, CMAQ was streamlined (Otte et al., 2005), by (1) reducing the system of chemical reactions to a limiting system for O_3 prediction, (2) reducing the number of vertical layers from 60 produced by NAM to 22, and (3) optimizing for the massively parallel computer system in NCEP operations. Further optimization may be needed to include a more complete set of chemical reactions for PM, or if more vertical resolution is required, or to increase coupling of weather and chemical models.

There is much interest in on-line approaches to integrate chemical modeling in parallel with weather prediction (see for example, Dabberdt et al., 2006). However, the required computational resources are considerably greater for full two-way coupling to the weather model than for the serial "off-line" approach currently used in operations. But there are also computational advantages in on-line approaches, gained by eliminating the need to store large volumes of weather data for subsequent applications, which permit the use of finer time-steps in weather information used for AQ predictions. Grell (2005) investigated the effect of varying time-steps of the predicted weather information on O_3 prediction; he found that reducing the time step frm one hour to about 10 minutes reduces (and improves) predicted O_3 concentrations. Impacts on weather prediction from on-line chemical approaches are realized through changes in, for example, aerosol distribution that affects simulated radiation fields. Grell (in progress) is studying the magnitude of this impact, and the effects of different frequency of feedback of predicted aerosol concentration fields on weather predictions.

Maintaining accuracy over expanding domains, with increasingly diverse pollution sources, weather patterns and topography/land-use, has proved difficult. Real-time evolutions' of predicted ground-level O_3 versus observations provided compiled by the US EPA's AIRNow program, and diagnostic evaluations with all other available information, from other networks and field campaign measurements (e.g. Mckeen et al., 2005), have shown that simple extensions of earlier Eastern US capabilities performed poorly over western US. Figure 3 compares performance test predictions for various configurations over 2005 and 2006, using a summary statistic for the near real-time evaluations. The summary tracks whether the prediction at monitor locations correctly matches daily exceedances of the 8-hour threshold of 85 ppb, commonly used by AQ forecasters in the US to issue O_3-based alerts. As compared against the target accuracy – fraction correct greater than 90%, shown by heavy lines in Figure 4 – it is quickly apparent that overall performance has improved. However, during 2006, there were frequent underpredictions of O_3 in western US, especially California, where forecast accuracy was much less than the domain-wide average.

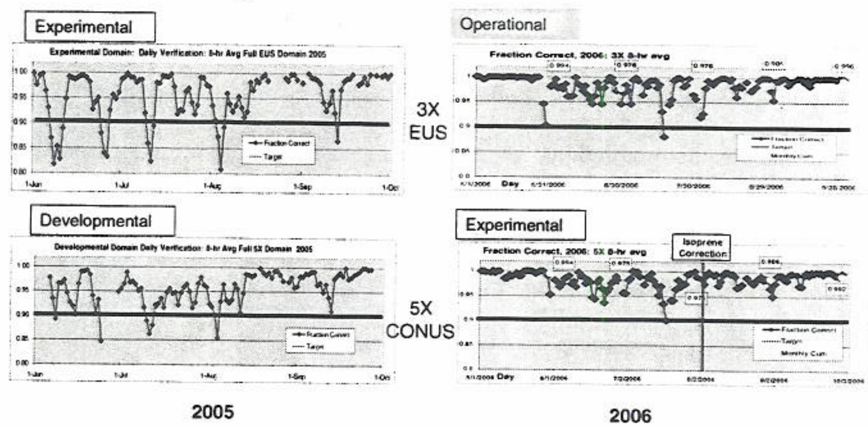

Fig. 3 Summary verification for ozone predictions for 2005 and 2006

We investigated several factors that can contribute to prediction accuracy in California, where complex terrain, large coastal urban areas, and unique weather patterns can exacerbate poor AQ: simulations of boundary layer dynamics, coupling of driving meteorological model physics to the AQ modules, emissions estimates, chemical boundary conditions, and simulations of reactive chemical processes. Extensive retrospective testing and analysis of alternative system configurations showed that better accuracy could be obtained with improvements in (1) emissions estimates from off-road mobile sources, (2) boundary-layer dynamics and (3) vertical mixing. These improvements are incorporated in the September 2007 operational expansion, to the CONUS.

As preliminary steps toward a quantitative capability for fine PM ($PM_{2.5}$) predictions, the NOAA team has tested and implemented predictions of smoke transport from large fires, while separately testing a developmental version of CMAQ extended from O_3 to include simulations of aerosols from emission inventories. The aerosol testing will be discussed further below. The smoke forecast capability incorporates the US Forest Service's estimates of emissions from burning wildfires along with several NOAA-developed capabilities, integrating NESDIS satellite information on location of wildfires with weather (NAM/WRF-NMM) mesoscale model) and smoke transport (HYSPLIT) models to produce daily predictions of smoke transport. Zeng and Kondragunta (2007) developed a technique for near-real time verification of predictions of the "footprint" of predicted smoke in the column based on satellite-derived aerosol optical depth. Forecast accuracy and reliability were monitored during experimental testing for nearly a year, with special attention to the warmer months, and successfully attained benchmark readiness criteria for operational deployment in March 2007. Predictions that include dust transport are in development.

Development and testing of other modules, in progress, is aimed at augmenting NOAA's AQ forecast capability to provide $PM_{2.5}$ forecasts with the same accuracy as the O_3 predictions. A version of CMAQ that is much more chemically comprehensive used for the O_3 predictions, but still uses the pollutant emissions inventory for chemical inputs, has been tested developmentally. Sample summary test verification with ground-based monitoring data, examined against a threshold of exceedance of 40 $\mu g/m^3$, for 24-hour averaged predictions is shown in Figure 5. Systematic differences in seasonal predictions, have been examined by Mathur et al. (2007) in diagnostic evaluations with speciated data. In summer, predicted total $PM_{2.5}$ is generally low as are secondary organic aerosols, consistent with omission of significant sources from wildfires and episodically, dust. Predicted winter totals are of the right order of magnitude, but overestimate some species, e.g. NO_3-, while underestimating others, e.g. organic carbon. Advanced chemical mechanisms that include more explicit contributions to secondary aerosols and nitrate cycling are being investigated. Improvements to the inventory-based primary contributions to $PM_{2.5}$ will also result in better estimates. However, given the uncertainties in both primary and precursor $PM_{2.5}$ source inputs from beyond the forecast domain, there is still much work to be done to increase prediction accuracy needed for a reliable quantitative prediction capability. Longer-term, improvements are planned for real-time chemical boundary conditions for the AQ forecast capability. NOAA is also planning to augment operational data assimilation to include available observations of chemical species.

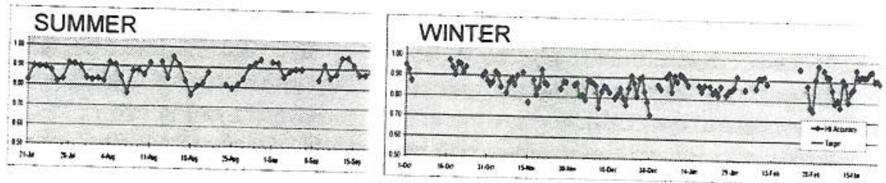

Fig. 4 Aerosol test verification samples

4. Summary

NOAA, in partnership with EPA is building a national AQ forecast capability. Via phased development, testing and operational implementation, NOAA's expanding capability provides AQ forecasters and the public with timely, accurate forecast information they need so that they can take actions to limit adverse effects of poor AQ.

Acknowledgments NOAA's AQ forecast implementation team is thanked for providing test results and analysis, both routine and for special. Our focus group of AQ forecasters, who work for state and local air agencies, are thanked for their continuing feedback based on their specialized expertise on AQ conditions.

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Discussion

B. Denby:

Do you couple real time observations and modelling in any may as a type of "now-cast" or plan to do so?

P. Davidson:

Real-time weather observations and fire locations are incorporated in the air quality predictions. Real-time monitoring data, with availability limited to ground-level ozone and particulate matter, are not included in the predictions. Plans call for ingest of real-time chemical observations. The Canadians have shown that ingest of real-time ozone monitoring data impacts the CHRONOS forecasts generally during the first six hours; accordingly NOAA's effort to develop chemical data assimilation capabilities are focussed on aerosol predictions, especially dust and smoke.

S. Hanna:

The criteria for forecast accuracy seem arbitrary (i.e., 90% accuracy of ozone concentration exceeding 85 ppb). How was the 90% number arrived at, and wouldn't it vary with concentration threshold (e.g., 100 ppb or 70 ppb instead of 85 ppb)?

P. Davidson:

There are many diagnostic criteria used in ongoing evaluations of prediction accuracy. For real-time verification required for operational forecasts, the 90% target described in the question was set according to the requirements of air quality forecasters, making sure to exceed persistence: Air quality forecasters in the US issue air quality alerts based on whether or not the next day's 8-hour average concentration of ground-level ozone exceeds 85 ppb. The target value would vary with the forecasters' requirements and persistence observed for different concentration thresholds.

R. San José:

Are you including real time and forecasting industrial emission data in your system? We do so in Spain at local level running MM5-CMAQ over cities and regions.

P. Davidson:

We include historically averaged values of industrial emission data in the predictions. We investigated the impacts on forecasts of using real-time emission recorded at power plants vs inventory records, and found surprisingly little sensitivity. Based on that result, we did not pursue the development necessary to include these data in the predictions.