Continuous, Near Real-Time Evaluation of Air Quality Models
An Approach for the Rapid Scientific Evolution of Modeling Systems

by Brian Eder, Robert Gilliam, George Pouliot, Rohit Mathur, and Jonathan Pleim

An evaluation of the Community Multi-scale Air Quality modeling system continuously and in near real-time.
Air quality models are required to address increasingly complex issues related to the representation of multiple pollutants species across multiple spatiotemporal scales, as well as those related to the design and implementation of more stringent National Ambient Air Quality Standards (NAAQS) designed to protect human health and the environment. Historically, most modeling groups have evaluated retrospective, often annual length model simulations, summarizing the performance using monthly or seasonal statistical summaries. While essential and informative, such an approach often masks finer scale temporal (e.g., diurnal to weekly) and spatial (e.g., meso to synoptic) variability in the earth–atmosphere system and, hence, air quality. In order to maintain state-of-the-science in the model, as well as the models’ ability to address emerging environmental needs, it is crucial that innovative evaluation approaches are developed and utilized that will allow for more rapid testing and hence more efficient evolution of the modeling system’s science.

Accordingly, the U.S. Environmental Protection Agency’s (EPA) National Exposure Research Laboratory (NERL) has performed and evaluated simulations of the Community Multi-scale Air Quality (CMAQ) model continuously and in near real-time (CMAQ_NRT) since 2014, following the protocol established when EPA was directly involved with the National Oceanic and Atmospheric Administration’s (NOAA) National Air Quality Forecast Capability (NAQFC), and recent recommendations published in the Bulletin of the American Meteorological Society.

**CMAQ**

The CMAQ modeling system is a powerful computational tool used for air quality management that links emissions models, meteorological models, and an air chemistry-transport model to simultaneously simulate multiple air pollutants, including ozone ($O_3$), fine particulate matter (PM$_{2.5}$), and a variety of air toxics. CMAQ provides detailed information about the emission, transport, and eventual fate of these air pollutants for any given area and for any specified emission or climate scenario. CMAQ has thousands of users in more than 50 countries and includes researchers, regulators, consultants, and forecasters in government, academia, and the private sector. States also use CMAQ to assess implementation actions needed to attain NAAQS and the U.S. National Weather Service uses CMAQ to produce daily, nationwide air quality forecasts.
Division scientists responsible for CMAQ meet bi-weekly to examine and critique the model’s daily performance while antecedent meteorological and air quality conditions remain familiar. This allows for immediate and ongoing analysis, thereby facilitating model evaluation (operational, performance, and diagnostic) of daily averaged PM\textsubscript{2.5} (mass only) and maximum 8-hr O\textsubscript{3} concentration. Additionally, using CMAQ\textsubscript{NRT} has facilitated numerous sensitivity analyses involving new science and has been used to inform field campaigns.

Observational data obtained from EPA’s Air Quality System (AQS) are used in the evaluation incorporating approximately 450 PM\textsubscript{2.5} mass and 950 O\textsubscript{3} monitors. The CMAQ\textsubscript{NRT} evaluation is limited to PM\textsubscript{2.5} mass because of the considerable lag time associated with the collection, processing, and dissemination of the speciated PM\textsubscript{2.5} observations. [Note: This does not preclude scientist from using CMAQ\textsubscript{NRT} to identify ideal case study periods and retrospectively evaluate its simulation of speciated PM\textsubscript{2.5} concentrations.]

Results are examined and discussed using a variety of statistical and visualization tools, a sampling of which is provided in the various case studies examined here. This compilation was designed to highlight case studies across pollutants (PM\textsubscript{2.5} and O\textsubscript{3} concentrations), years (2015, 2016, and 2017) and meteorological, chemical, and emissions processes. Some of the issues have been resolved while others are the subject of ongoing research.

Figure 2. Elevated PM\textsubscript{2.5} concentrations (µg/m\textsuperscript{3}) associated with cold pool development in the Great Salt Lake Valley near Provo, Utah on February 1, 2017.

Figure 3. Excessive O\textsubscript{3} concentrations (ppb) over southern Lake Michigan on June 10, 2016.
Difficulty Resolving Winter Cold Pools within Valleys

When simulating with its 12-km horizontal grid resolution, CMAQ\textsubscript{NRT} often displays difficulty in capturing the finer details of boundary layer meteorology located in valleys with highly variable terrain. This limitation, which impacts simulation of both PM\textsubscript{2.5} and O\textsubscript{3}, is exacerbated under certain meteorological regimes as identified by the CMAQ\textsubscript{NRT} simulations. Such regimes tend to occur during the cold months, when areas are influenced by continental Polar (cP) anticyclones. This is especially true when snow cover is extensive, as illustrated in Figure 2, which shows the model greatly underpredicting PM\textsubscript{2.5} concentrations for a monitor located in the Great Salt Lake Valley near Provo, Utah for February 1, 2017. Considerable interest in “cold pool” events has arisen lately prompting field studies in Salt Lake City and the Uinta Basin in Utah. Recent studies suggest that finer model resolution is needed to adequately capture the complex meteorological processes that occur in these valleys.

### Table 1

Statistics associated with a sensitivity analysis using updated organic aerosol source strength and partitioning in the simulation of PM\textsubscript{2.5} (µg/m\textsuperscript{3}) across the contiguous United States for the week of January 25–31, 2017.

<table>
<thead>
<tr>
<th>Model Configuration</th>
<th>Σ paired n</th>
<th>Mean Obs.</th>
<th>Mean CMAQ</th>
<th>RMSE</th>
<th>Mean Bias</th>
<th>r</th>
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<tbody>
<tr>
<td>Base CMAQ\textsubscript{NRT}</td>
<td>3006</td>
<td>7.6</td>
<td>8.8</td>
<td>6.6</td>
<td>+1.1</td>
<td>0.44</td>
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<td>Updated CMAQ\textsubscript{NRT}</td>
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<td>7.5</td>
<td>5.6</td>
<td>-0.1</td>
<td>0.47</td>
</tr>
</tbody>
</table>

### Case Studies

#### Excessive Windblown Dust Emissions

Windblown dust emissions within the modeling system were often exceptionally large, especially in the western United States during the winter and spring months. CMAQ\textsubscript{NRT} demonstrated one such event in southern Nevada and California on January 31, 2016 (see Figure 1), where hourly PM\textsubscript{2.5} concentrations attributable mainly to emissions of soil and “PM-other” exceeded 2,500 µg/m\textsuperscript{3}. Accordingly, Foroutan et al. developed and integrated within CMAQ, a physics-based windblown dust emission parameterization that greatly improved emission estimates. Sensitivities using the CMAQ\textsubscript{NRT} showed that the new scheme has greatly reduced the modeled emissions and is capable of more accurately capturing the spatial and temporal characteristics of dust events.

#### Figure 4

Excessive PM\textsubscript{2.5} concentrations (µg/m\textsuperscript{3}) attributable to miss-allocated residential wood combustion emissions on February 1, 2014. Hourly simulated concentrations for Brooklyn, NY.
resolution, more accurate snow cover, as well as adjustments to microphysics schemes are needed to properly simulate this terrain induced phenomenon. Sensitivities exploring the expectant improvement of higher resolution (e.g., 4 and 1 km) CMAQ \(_{NRT}\) simulations and other model changes under such scenarios are planned.

**Elevated O\(_3\) Concentrations over Great Lakes**

Under certain meteorological regimes, CMAQ \(_{NRT}\) simulates very high O\(_3\) concentrations over the Great Lakes (>125 parts per billion [ppb] over Lake Michigan in this example seen in Figure 3). While somewhat elevated concentrations can be expected (due mainly to limited boundary layer growth over the Lakes) concentrations this high are not supported by recent literature. Field campaigns, such as the Lake Michigan Ozone Study (2017) could provide much needed data for evaluating the model under such scenarios. Additionally, further research is planned determine whether simulations might be improved by refining the representation of localized lake and/or shoreline meteorology.

**Updated Organic Aerosol Source Strength and Partitioning**

A sensitivity analysis utilizing CMAQ \(_{NRT}\) helped corroborate the importance of accounting for the semivolatile partitioning of primary organic aerosol (POA) compounds consistent with experimentally derived parameterizations. Also included in the sensitivity was a new surrogate species, potential-combustion secondary organic aerosol (pcSOA), which provides a cumulative representation of the SOA from combustion sources. Summary statistics for the period January 25–31, 2017, are provided in Table 1, illustrating the improvement in model performance associated with these changes which were incorporated into the most recent release of CMAQ (v5.2).

**Residential Wood Combustion**

The residential wood combustion (RWC) sector of EPA’s National Emission Inventory (2011) was greatly overestimated in high-density urban areas because the emissions were based on metropolitan statistical areas (MSA) populations. The inventory within each MSA did not take into account the dearth of heating attributable to RWC in very highly populated areas such as New York City. Numerous examples of this miss-allocation were discovered by CMAQ \(_{NRT}\), including results shown in Figure 4, which illustrate exceptionally large hourly PM\(_{2.5}\) concentrations (approaching 200 µg/m\(^3\)) mainly attributable to elemental carbon (EC), organic carbon (OC), and “PM-other”–CMAQ species that indicate RWC in Brooklyn, New York on February 1, 2014. Version 2 of EPA’s 2011 National Emissions Inventory (NEI) eliminated this high-bias by improving the allocation of RWC emissions.

**Independence Day Pyrotechnics**

Some of the highest PM\(_{2.5}\) concentrations in the United States occur during the late evening/early morning hours after Independence Day celebrations. The impact of the widespread use of pyrotechnics (which are not represented in EPA’s NEI) has been well documented each of the three years that the division has been running CMAQ \(_{NRT}\). An example of which is provided in Figure 5, showing very high hourly PM\(_{2.5}\) concentrations across many AQS sites that are obviously not captured by the model. A typical signature of the pyrotechnics plume is also shown impacting a site near Simi Valley, CA. Future studies investigating the influence of such celebrations...
(which are also seen, though to a lesser degree for New Year’s Day) would benefit from the preliminary analysis provided by CMAQ\textsubscript{NRT}.

**Summary**

Running an air quality model such as CMAQ continuously and in near real-time has proven advantageous for numerous reasons. As shown, such an approach has led to the identification, and when possible, the resolution of numerous issues that conventional evaluation techniques (e.g., those involving retrospective, often long-term, simulations) would likely miss. Specifically, CMAQ\textsubscript{NRT} has helped identify meteorological (e.g., boundary layer, transport), chemical (e.g., semi-volatile partitioning of POA), and emission (e.g., RWC, wind-blown dust) issues associated with the modeling system. Resolution of these and other issues not discussed here has been incorporated into the latest releases of CMAQ, including Version 5.1, released in 2015 and highlighted in *EM* and more recently Version 5.2 to be released this year.

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**References**


**In Next Month’s Issue…**

**Water Management Associated with Oil and Gas Development and Production**

The development and production of oil and gas not only requires water, but also produces water. In fact, in some cases, an oil or gas well produces greater volumes of water than the extracted oil or gas. Articles in the August issue will address advancements in technologies and understanding of water quantity and quality and viable recycling and reuse opportunities to be both good stewards of water resources, as well as be protective of human health and the environment.