Regional Photochemical Modeling - Obstacles and Challenges

Extended Abstract No. 33594

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INTRODUCTION

Regional photochemical modeling is becoming an increasingly important technique to evaluate ozone and secondary particulate matter less than 2.5 microns (PM$_{2.5}$) impacts from single sources. Photochemical models are defined as numerical models that simulate the emission, chemical transformation, transport, and deposition of gases and aerosols. Recent policies have triggered a new wave of modeling needs potentially requiring industry to perform regional modeling for evaluating ozone and secondary PM$_{2.5}$ in the absence of any non-draft U.S. EPA guidance and recommendations. Although regional photochemical modeling has been evolving for the past decade, the focus of these modeling studies has been on multiple sources located over a larger scale area.

Lack of guidance and uncertainty in the ozone significance threshold for evaluating single source industrial impacts dates back at least three decades. According to a U.S. EPA presentation in May 2005, Joseph Cannon (Assistant Administrator of the U.S. EPA Air and Radiation) corresponded with a law firm in Dallas to address a Prevention of Significant Deterioration (PSD) question for a proposed plant in Texas. A letter from the law firm summarized the meetings in Durham, North Carolina and Washington D.C. with the U.S. EPA and indicated the U.S. EPA was considering 0.3 ppb as the ozone significance threshold, but no definite “significance level” was decided. Mr. Cannon’s response was to confirm the balance of the law firm’s understanding on this issue. The correspondence seemed to confirm the U.S. EPA was considering using 0.3 ppb as the significance threshold, but had not made a determination on the issue.

The U.S. EPA recently granted a Sierra Club petition with a commitment to update 40 CFR Part 51 Appendix W “Guideline on Air Quality Models” to address ozone and secondary PM$_{2.5}$ impacts under the New Source Review (NSR) and PSD programs. According to a U.S. EPA presentation in July 2013, the U.S. EPA will provide more guidance on an appropriate approach for model application for secondary impact permit assessments. To date, however, the U.S. EPA has not yet determined a significance threshold for evaluating ozone impacts from single sources, nor has it developed a strict guidance for metrics to use for assessing single source ozone impacts. Rather, the determination of metrics, and the interpretation of these metrics, is handled on a case-by-case basis from the U.S. EPA regional offices and state agencies. Because of the lack of U.S. EPA guidance, most single source impact evaluations rely on the 2007 U.S. EPA
“Guidance on the use of Models and other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM$_{2.5}$, and Regional Haze” as a basis for the analysis. This methodology involves using a photochemical model, such as the Community Multi-Scale Air Quality System (CMAQ) or Comprehensive Air Quality Models with Extension (CAMx), to evaluate ozone impacts using the relative response factor (RRF) method.

In addition to ozone modeling, photochemical modeling is becoming an increasingly important technique to evaluate air toxics, visibility impairment, secondary PM$_{2.5}$ formation, and inter-pollutant trading ratios. The Texas Commission for Environmental Quality (TCEQ) recently released two guidance documents on procedures to perform photochemical modeling for the use of inter-pollutant, inter-basin trading ratios. The U.S. EPA PM$_{2.5}$ draft modeling guidance released in March 2013 suggests photochemical modeling for secondary formation of PM$_{2.5}$ will be required in certain cases. These recent events have triggered a new wave of photochemical modeling needs.

PHOTOCHEMICAL MODELING

By definition, photochemical models are defined as numerical models that simulate the emissions, chemical transformation, transport, and deposition of gases and aerosols. The first generation models developed in the 1970s and 1980s primarily included single source dispersion models such as Gaussian plume models and chemical box models. There has been an exponential increase in model complexity since the first generation models. The advances in computer technology, availability of affordable processing, and advances in atmospheric science, led to the development of first multi-source photochemical transformation and transport models. These second generation air quality models, such as the Urban Airshed Model (UAM) and Regional Modeling System for Aerosols Depositions (REMSAD), were designed to calculate concentration of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentration over regional scales. Other models developed during the same time were the Regional Oxidant Model (ROM), Regional Acid Deposition Model, and Sulfur Transport and Emissions Model.

The Clean Air Act Amendments of 1990 identified a wide range of additional issues such as visibility, fine and coarse particles, indirect exposure to toxic pollutants, and nutrient deposition to water bodies. To address these additional issues and increased modeling needs, third generation air quality models were developed. These modeling systems include the Community Multi-Scale Air Quality System (CMAQ) and Comprehensive Air Quality Models with Extension (CAMx) among others. These models are community based models described as:

- modular for greater flexibility and integration of new science;
- completely portable amongst all UNIX/Linux based open source platforms;
- open source and accessible to everyone; and
- open for development by the modeling community.

Additionally, to address the complex relationship between pollutants, these models address air quality from a one-atmosphere multi-pollutant perspective. Conceptually, the one-atmosphere approach must address multi-pollutant and multi-scale processes. This approach should integrate...
influence of interactions at different dynamic scales and among multi-pollutants. For example, a typical aerosol cycle can have the following multi-scale processes:

- dry deposition;
- wet deposition;
- acid precipitation;
- gas-phase chemistry and aqueous chemistry; and
- chemical production, nucleation, condensation, depositional growth, dissolution, evaporation, and washout.

All of these processes are interacting and affecting each other. These processes need to be addressed, and the third generation photochemical models are designed to do so.

**CHALLENGES**

Elevated ground level ozone concentrations in urban areas are a result of atmospheric photochemical reactions among various chemical species, which occur under favorable meteorological conditions (e.g., high ground level temperature, light winds, and abundant sunlight). These chemical species are generated from several key precursors including nitrogen oxides (NOx) and volatile organic compound (VOC) emissions from both anthropogenic (e.g., mobile and stationary sources) and natural sources (e.g., trees). These precursors may come from local sources or be transported into the area from distant sources as far as hundreds of miles away. Pursuant to 40 CFR 52.21, a proposed project with a project increase of VOC or NOx emissions in excess of 100 tpy triggers an ambient ozone impact analysis for the project.

Use of the 2007 U.S. EPA attainment guidance for evaluating a project’s single source impact is not entirely appropriate for several reasons. The 2007 U.S. EPA attainment guidance recommends using the photochemical model in a “relative” rather than “absolute” sense for the modeled attainment test. To do so, relative response factors (RRFs) are computed by taking the ratio of the model’s future to current (i.e., baseline) predictions at ambient monitors. The guidance recommends using only days with a daily maximum 8-hour average baseline modeled ozone value greater than 85 ppb (i.e., minimum concentration threshold), but down to as low as 70 ppb, to calculate RRFs. This approach does not directly correspond to the proper assessment of a single source’s impact because it does not consider all days and does not appropriately compare to the National Ambient Air Quality Standard (NAAQS) as do single source PSD impact methodologies for other pollutants. Next, future ozone and/or PM2.5 concentrations are estimated at existing monitoring sites by multiplying a modeled RRF at locations “near” each monitor by the observation-based, monitor-specific, “baseline” design value. The resulting predicted “future concentrations” are compared to the NAAQS. This methodology does not reflect the 8-hour ozone design values and should not be interpreted as an indication that a facility will cause or contribute to an exceedance of the 8-hour NAAQS because the purpose of this guidance is to provide U.S. EPA Regional, State, and Tribal air quality management authorities on how to prepare attainment demonstrations and not on how to address single source impacts.

Second, the U.S. EPA has not set a *de minimis* concentration level for ozone impacts. Similarly, the U.S. EPA has not set *de minimis* levels for one hour NO2 or SO2 impacts. However, the U.S. EPA published guidance for modeling of one-hour NO2 and SO2, which suggests an interim
significant impact level (SIL) to be set at 4% of the applicable NAAQS. If this suggested 4% level is applied to the 8-hour ozone 2008 NAAQS of 75 ppb, a SIL of 3.0 ppb is the result. Similarly, the SIL/NAAQS ratio for other pollutants on a short-term averaging period are examined in Table 1 to determine an appropriate 8-hour ozone SIL. Table 1 shows the NAAQS, SIL, and corresponding SIL/NAAQS ratio for PM$_{10}$ (24-hour), PM$_{2.5}$ (24-hour), and CO (8-hour and 1-hour). The SIL/NAAQS ratio range for these pollutants is from 3.3% to 5%. This range corresponds to a SIL range of 2.5 ppb to 3.8 ppb when applied to the 8-hour ozone 2008 NAAQS. If the U.S. EPA were to establish a SIL for ozone, single sources would have the opportunity to reasonably conclude that simulated impacts that are equal to or lower than the SIL would not likely be considered significant.

Table 1. The National Ambient Air Quality Standard (NAAQS), Significant Impact Level (SIL), and corresponding SIL/NAAQS Ratio for Short-term Averaging Period Pollutants

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>NAAQS ($\mu g/m^3$)</th>
<th>SIL ($\mu g/m^3$)</th>
<th>SIL/NAAQS Ratio (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM$_{10}$ (24-hour)</td>
<td>150</td>
<td>5</td>
<td>3.3</td>
</tr>
<tr>
<td>PM$_{2.5}$ (24-hour)</td>
<td>35</td>
<td>1.2</td>
<td>3.4</td>
</tr>
<tr>
<td>CO (8-hour)</td>
<td>10,000</td>
<td>500</td>
<td>5.0</td>
</tr>
<tr>
<td>CO (1-hour)</td>
<td>40,000</td>
<td>2,000</td>
<td>5.0</td>
</tr>
</tbody>
</table>

In addition to the issues associated with the lack of existing guidance and established SIL, a photochemical model, such as CAMx or CMAQ, is in actuality just one complex component of a modeling system. For example, CAMx and CMAQ inputs are developed using independent third-party models and processing tools such as the:

- Weather Research Forecasting (WRF) or Fifth-Generation Pennsylvania State/National Center for Atmospheric Research (MM5) models for meteorological data,
- MOBILE6 or Motor Vehicle Emission Simulator (MOVES) for mobile source emission inventories,
- NONROAD model (NRM) for non-road vehicle inventories, and
- Model of Emissions of Gases and Aerosols from Nature (MEGAN) or
- Biogenic Emission Inventory System (BEIS)

for characterizing meteorology, emissions, and various other environmental conditions (land cover, radiative/photolysis properties, and initial/boundary conditions).

Moreover, interface programs are needed to translate the products of each of these models/processors into the specific input fields and formats required by CAMx and CMAQ. For example, the Sparse Matrix Kernel Emission (SMOKE) modeling system is required to create gridded, speciated, hourly emissions for input into the photochemical model. SMOKE transforms the output from other emission inventory programs into input for CMAQ (or CAMx), Similarly, the Meteorology-Chemistry Interface Processor (MCIP) converts WRF (or MM5) output files into CMAQ-ready meteorological files by calculating parameters such as Monin-Obukhov length or dry deposition velocities not provided by WRF. Additional programs are used to post-process the concentration fields, develop model performance statistics and measures, manipulate probing tool output into various reportable formats, and further translate raw results into forms necessary
for regulatory purposes after the air quality simulation is completed. Extensive experience, knowledge, time, and most importantly resources in the form of modeling clusters are required to use these components of the CAMx (or CMAQ) modeling system.

For the reasons described above, photochemical modeling requires an extensive amount of computing power compared to other U.S. EPA approved models (e.g., AERMOD and CALPUFF) used for PSD purposes. A simple model application with 100 columns x 100 rows x 25 layers results in 250,000 grid cells. The simple Carbon Bond 6 mechanism contains 79 species and 94 reactions. Therefore, the number of differential equations to be solved by computer per model output time setup is 19,750,000. To run only one day worth of model runs in this scenario will require a model to solve 474 million equations. This data intensive model run can only be completed on a Linux cluster with multiple nodes and multiple processors in each node.

Furthermore, photochemical modeling projects are very expensive. If a facility is fortunate enough to be located in state that is required to conduct State Implementation Plan (SIP) photochemical modeling and the state makes these files available to the public (e.g., Louisiana and Texas), then the facility has the opportunity to utilize these files for its ambient ozone and secondary PM$_{2.5}$ impact analysis. These projects might range from $50,000 to $100,000. If photochemical modeling files are not available, a very large financial burden is placed on the facility. These projects can cost up to several hundred thousand dollars.

**SUMMARY**

Although regional photochemical modeling has been evolving for the past decade, the focus of the modeling studies has been on the larger scale with multiple sources. Recent policies and draft guidance have triggered a new wave of modeling needs that requires industry to perform regional modeling on a much smaller scale (e.g., county or nonattainment area level). This paper provides an overview of the third generation air quality modeling systems and its components including the CMAQ and CAMx models. The paper focuses on the need and importance for regional modeling guidance from regulatory agencies, the obstacles in performing the modeling, and the future challenges faced by industry to perform regional scale modeling analyses using such modeling systems.

**REFERENCES**


