Evaluation of Options for Addressing Secondary PM_{2.5} and Ozone Formation

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Overview

- Timeline and reasoning
- Regulatory drivers in the U.S.
- Emerging approaches
  - Qualitative
  - Screening
  - More advanced modeling
  - Comprehensive photochemical grid modeling with reusable modeling platforms
Regulatory Drivers

• Inert pollutants properly handled with air dispersion models
• Pollutants with in-transit chemistry more difficult:
  • Total PM$_{2.5}$ = direct PM$_{2.5}$ + secondary PM$_{2.5}$ \{particulate sulfates + particulate nitrates + ambient environment\}
  • Ozone = NOx + VOC + \{ambient environment\}
• Known health effects of PM$_{2.5}$ and ozone
  • Lowering ambient air quality standards
• Regional Haze Rule \(\rightarrow\) reach natural visibility conditions by 2064
• These overarching factors have been pushing forward the need to quantify secondary formation on a more regular basis
Where We Are Now

• In response to Sierra Club lawsuit, EPA agreed to require sources to address ‘project level’ emissions of secondary PM$_{2.5}$ and ozone in permitting efforts
  • Changes to US EPA federal modeling guidance (Guideline on Air Quality Models, Appendix W)
• Implementation Considerations:
  • Balance between simplistically conservative and science project
  • Need to build experience within the regulated community
  • Identification of reasonable modeling approaches and data needs
  • Build a “threshold” for routine approval
Known Science – PM$_{2.5}$

- Total PM$_{2.5}$ = Direct PM$_{2.5}$ + secondarily formed PM$_{2.5}$
  - Direct assumed to be inert and easy to model
  - Secondary PM$_{2.5}$ is the formation of particulate sulfate and particulate from emitted SO$_2$ and NOx into the ambient environment
  - Ambient environment function of many variables –
    - Ammonia, meteorology, competing sources
Known Science - Ozone

- Ozone is the result of photochemical reactions involving NOx and VOC emitted into the ambient environment
  - Chemistry is known to be complex and non-linear
  - Proper speciation of source VOC emissions
  - Ambient environment important
  - A lot of our understanding of ozone is based on summer, urban environments with traffic as primary drives
  - Any model needs to concurrently integrate all variables then march forward in time  → difficult!
Emerging Science

• Both PM$_{2.5}$ and ozone issues have real exceptions to known science
  • Capital Region / Red Deer winter PM$_{2.5}$
  • Intermountain US West winter ozone
Approaches

- Qualitative
  - Monitoring data; emission trends; ambient environment
- Simple modeling
  - Add SO$_2$ and NOx emissions to direct PM$_{2.5}$ emissions
  - Box models or EKMA approach for ozone
- More advanced modeling
  - CALPUFF; SCICHEM
    - CALPUFF cannot model ozone
- Photochemical grid modeling
  - Leverage existing modeling platforms
  - Conduct new modeling for specific source

Our focus
## Model Inter-comparisons

<table>
<thead>
<tr>
<th>Component</th>
<th>CALPUFF</th>
<th>SCICHEM</th>
<th>CAMx</th>
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<tbody>
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<td><strong>Status</strong></td>
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<td>Ramboll ENVIRON</td>
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<td><strong>EPA Regulatory Status</strong></td>
<td>Proposed de-listing as EPA approved model; can be used for screening with approval</td>
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<td>Days to weeks</td>
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Evaluations of SCICHEM, CALPUFF, & CAMx

From “Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments” September 2012

- SCICHEM with observed meteorology
- SCICHEM with WRF/MMIF meteorology
- CAMx with MEGAN biogenic emissions
- CAMx with BEIS biogenic emissions
- CALPUFF v5.8 with CALMET meteorology
- CALPUFF v5.8 with WRF/MMIF meteorology

<table>
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<tr>
<th>Transect</th>
<th>Plume ID</th>
<th>Downwind Distance (km)</th>
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<th>CAMx</th>
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Observed and simulated cross-wind plume concentrations of $SO_2$ (ppb) for Traverse 3 at 11 km downwind (taken from “Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments”)

**SCICHEM w WRF/MMIF**

**CAMx**

**CALPUFF**
Observed and simulated cross-wind plume concentrations of NO$_2$ (ppb) for Traverse 3 at 11 km downwind (taken from “Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments”)

Note that NOx is reported for CALPUFF
Observed and simulated cross-wind plume concentrations of $O_3$ (ppb) for Traverse 3 at 11 km downwind (taken from “Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments”)

SCICHEM w WRF/MMIF

CAMx
Observed and simulated cross-wind plume concentrations of \( \text{SO}_2 \) (ppb) for Traverse 8 at 31 km downwind (taken from “Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments”)
Observed and simulated cross-wind plume concentrations of NO$_2$ (ppb) for Traverse 8 at 31 km downwind (taken from “Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments”)

Note that NOx is reported for CALPUFF
Observed and simulated cross-wind plume concentrations of O$_3$ (ppb) for Traverse 8 at 31 km downwind (taken from “Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments”)

SCICHEM w/obs, MMIF similar

CAMx
Single Source Modeling for Ozone and PM$_{2.5}$
An Evolving Effort
Leveraging Existing Platforms

- “Projects would NOT need to generate complex model runs.
- Use a threshold approach
- Summarized in December USEPA 2016 guidance
  - “Modeled Emission Rates for Precursor Pollutants” or MERPs guidance
  - PM$_{2.5}$
  - Ozone
Source Locations Modelled by EPA
MERPs

- Modelling varied:
  - Stack heights (high and low)
  - Emission levels of precursors (one precursor modelled at a time)
  - Spatial distribution takes into account local and regional-scale influences
- Results used to:
  - Determine emission thresholds below which ozone and secondary formation is ‘insignificant’
  - Region-specific modelled response for precursor, i.e., $X \text{ tpy of precursor } \rightarrow Y \mu g/m^3$
  - Can use worst-case or “representative” results for a particular project
  - Or use modeling files (provided by EPA) to do own modeling
MERPs

• This approach is:
  • Easy
  • Efficient
  • Based on peer review
  • Use worst-case or representative results
  • Provides a reusable modeling platform

• Only available for continental U.S.
  • Could be extended to Canada?
Conclusions

- CALPUFF performance degraded with distance
- “Both CAMx and SCICHEM show skill in modeling ozone titration and formation effects within the ... plume.”
  - CAMx shows sensitivity to background VOCs
  - SCICHEM shows sensitivity to meteorological data
- MERPs as a screening tool for ozone and PM$_{2.5}$