CALPUFF Near-field Validation

Roger W. Brode
U.S. EPA/OAQPS
Air Quality Modeling Group

10th Conference on Air Quality Modeling
March 13, 2012
Research Triangle Park, NC
Outline

• Regulatory status of CALPUFF for near-field applications (nominally within 50km)
• August 2008 Clarification Memo and Technical Issues Memo
• History of CALPUFF near-field validations
• CALPUFF validation study conducted for NJ 126 petition
CALPUFF Near-field Clarification Memorandum

• Summary of Key Points:
  – The EPA-preferred model for near-field regulatory applications (less than 50 kilometers) for simple and complex terrain is AERMOD. The AERMOD model should be used for all near-field regulatory applications, unless an adequate determination is made that AERMOD is not appropriate for that application or is clearly less appropriate than an alternative model. [See paragraph 4.2.2(b) of Appendix W – “For a wide range of regulatory applications in all types of terrain, the recommended model is AERMOD.”]

  – CALPUFF is not the EPA-preferred model for near-field applications, but may be considered as an alternative model on a case-by-case basis for near-field applications involving “complex winds,” subject to approval by the reviewing authority. The approval of CALPUFF for near-field regulatory applications should be based on case-specific justification, including necessary documentation and an adequate determination that AERMOD is not appropriate or clearly less appropriate than CALPUFF. Generalized approval of CALPUFF for near-field applications based on reference to other cases where CALPUFF has been approved for near-field use is not acceptable, unless such cases are similar enough to the application under review to be applicable, and are adequately documented to support that determination. [See paragraph 7.2.8(a) of Appendix W – “the CALPUFF modeling system (described in Appendix A) may be applied on a case-by-case basis for air quality estimates in such complex non-steady-state meteorological conditions.”]
CALPUFF Near-field Clarification Memorandum

• From Preamble to April 2003 FR Notice promulgating CALPUFF:
  – “We will require approval to be obtained prior to accepting CALPUFF for complex wind situations, as this will ensure that a protocol is agreed to between the parties involved, and that all are willing to accept the results as binding. As experience is gained in using CALPUFF for complex wind situations, acceptance will become clear and those cases that are problematic will be better identified.” (pp. 18441-2)
CALPUFF Near-field Clarification Memorandum

• From Section 7.2.8 of Appendix W:
  – “The setup and application of the model should be determined in consultation with the appropriate reviewing authority (paragraph 3.0(b)) consistent with limitations of paragraph 3.2.2(e).”
  – Reference to paragraph 3.2.2(e) places CALPUFF in the status of an alternative model.
• Paragraph 3.2.2(e) of Appendix W:

“e. Finally, for condition (3) in paragraph (b) of this subsection [preferred model is less appropriate for the specific application, or there is no preferred model], an alternative refined model may be used provided that:

i. The model has received a scientific peer review;

ii. The model can be demonstrated to be applicable to the problem on a theoretical basis;

iii. The data bases which are necessary to perform the analysis are available and adequate;

iv. Appropriate performance evaluations of the model have shown that the model is not biased toward underestimates; and

v. A protocol on methods and procedures to be followed has been established.”
CALPUFF Near-field Clarification Memorandum

• Summary of main steps:
  1) a determination that treatment of complex winds is critical to estimating design concentrations;
  2) a determination that the preferred model is not appropriate or less appropriate than CALPUFF; and
  3) a demonstration that the five criteria listed in paragraph 3.2.2(e) for use of an alternative model are adequately addressed.

• Each of these steps involves case-specific considerations
Examples of Complex Winds

• Examples of complex winds are described in paragraph 7.2.8(a) of Appendix W:
  – “a. Inhomogeneous Local Winds. In many parts of the United States, the ground is neither flat nor is the ground cover (or land use) uniform. These geographical variations can generate local winds and circulations, and modify the prevailing ambient winds and circulations. Geographic effects are most apparent when the ambient winds are light or calm. In general these geographically induced wind circulation effects are named after the source location of the winds, e.g., lake and sea breezes, and mountain and valley winds. In very rugged hilly or mountainous terrain, along coastlines, or near large land use variations, the characterization of the winds is a balance of various forces, such that the assumptions of steady-state straight-line transport both in time and space are inappropriate.”
Complex Winds – Performance Evaluations

• CALPUFF modeling system performance for near-field complex wind applications is not well-documented

• IWAQM Phase 2 report includes some CALPUFF evaluation results for Kincaid (flat terrain) and Lovett (complex terrain)

• Evaluation results for Lovett show good performance
CALPUFF Lovett Evaluation Results from IWAQM Phase 2 Report

Figure 28. Q-Q plots for Lovett, comparing observed surface concentration values of $SO_2$ with simulation results CALPUFF(4.07) and CTDPLUS.
Complex Winds – Performance Evaluations

• However, CALPUFF was applied with CTDMPLUS met inputs, bypassing CALMET
• This is not consistent with motivation for CALPUFF near-field applications under paragraph 7.2.8 of Appendix W, which is to “fully treat the time and space variations of meteorology effects on transport and dispersion.”
• Therefore, these evaluation results are not relevant to near-field applications under paragraph 7.2.8 of Appendix W
NJDEP CALPUFF Validation

- New Jersey Department of Environmental Protection (NJDEP) submitted a CALPUFF near-field validation study using Martin’s Creek field study in support of a CAA Section 126 petition against the Portland Generating Station (PGS) under the 1-hour SO$_2$ NAAQS:
  - Section 126 of CAA addresses interstate transport that may significantly contribute to non-attainment or interfere with maintenance of a NAAQS in a downwind state
  - NJDEP claimed that the validation study demonstrates “CALPUFF performed better and produced predictions of greater accuracy than AERMOD”
  - PGS was not the main focus of Martin’s Creek field study, but was included as one of the background sources
  - NJDEP also claimed that CALPUFF was more appropriate than AERMOD due to the influence of “complex winds” per Section 7.2.8 of Appendix W
NJDEP CALPUFF Validation

• Determination of whether CALPUFF validation study demonstrated whether CALPUFF performed better than AERMOD was important in EPA’s response:
  – CALPUFF modeling results submitted by NJDEP for PGS were much higher than AERMOD results;
  – Acceptance of CALPUFF results as the basis for EPA’s response would have required a much lower emission threshold to eliminate PGS’ significant contribution to nonattainment or interference with maintenance of the 1-hour SO$_2$ NAAQS in New Jersey
Martin’s Creek (MCR) Field Study

Location of SO2 sources, monitors and meteorological stations used in the model validation study
NJDEP CALPUFF Validation

• EPA identified several issues with the NJDEP evaluation protocol, including:
  • Varying the number of values (N) in determining Robust Highest Concentrations (RHCs);
  • Inclusion of results for AMS8 monitor which was intended and used only for estimating background concentrations in previous MCR evaluations;
  • Residual analyses based on ranked distributions of modeled and observed concentrations;
  • Details regarding these issues are addressed in the Technical Support Documents (TSDs) for the proposed and final rules, and final RTC document
NJDEP Q-Q Plots for MCR Study
NJDEP Boot Analysis Results

Network 1-Hour Peak Time Series Fractional Bias with 95% Confidence Limits

CALPUFF

AERMOD
Cox-Tikvart Protocol Results

Martin's Creek SO2 - AERMOD vs. CALPUFF (w/o PRM)
Model Comparison Measure - With AMS8
With 90% Confidence Limits
Initial Assessment

• An initial assessment of the Q-Q plots, Boot analysis program results, and Cox-Tikvart protocol suggest similar performance for CALPUFF and AERMOD for MCR field study.

• Since the confidence intervals on Boot analysis and Cox-Tikvart results overlap, the differences in model performance are not statistically significant.

• Similarity of these evaluation results does not support the claim that CALPUFF performs better than AERMOD for this application.
Further Assessments

• Review of CALPUFF input files indicated that the PRIME downwash algorithm was not used in NJDEP’s CALPUFF modeling

• Downwash influences from nearby cooling towers on MCR stacks was accounted for in AERMOD evaluation based on PRIME

• Use of PRIME downwash algorithm in CALPUFF degrades CALPUFF performance
Impact of PRIME on CALPUFF

Q-Q Plot of 1-hr Network-wide SO2 for Martin's Creek w/PRIME for CALPUFF

- **Predicted Conc (ug/m3)**
- **Observed Conc (ug/m3)**

Legend:
- **AERMOD**
- **CALPUFF PRIME**
- **CALPUFF ISC-Type**
Impact of PRIME on CALPUFF

Martin's Creek SO2 - AERMOD vs. CALPUFF-PRM
Model Comparison Measure - With AMS8
With 90% Confidence Limits

Model Comparison Measure (MCM)

Martin's Creek SO2 - AERMOD vs. CALPUFF-PRM
Model Comparison Measure - Without AMS8
With 90% Confidence Limits

Model Comparison Measure (MCM)
Additional Model-to-Monitor Comparisons

• NJDEP installed an SO$_2$ ambient monitor at Columbia Lake, about 2km NE of PGS in Sept. 2010;

• Columbia monitoring data shows numerous exceedances of 1-hr SO$_2$ NAAQS, with 99$^{th}$-percentile daily maximum 1-hr value for first year of 136 ppb (355.4 ug/m$^3$).
Columbia Monitor Location
Columbia Lake - Sept. 23, 2010 to Feb. 17, 2011
Portland Model-to-Monitor Comparisons

- Model-to-monitor comparisons of Portland impacts on the nearby Columbia, NJ monitor were conducted as part of the NJ 126 petition assessment.

- The following table compares 10 highest observed and predicted daily maximum 1-hour SO2 concentrations:
  - Observed data are based on Sept. 23, 2010 – Sept. 22, 2011
  - AERMOD results based on site-specific met data from July 1, 1993 – June 30, 1994; with representative emissions
  - CALPUFF modeled data based on three sets of met data included in NJ 126 petition; with same emissions as AERMOD;
  - Despite significant difference in data periods, distribution of the highest daily maximum 1-hour values is very similar for AERMOD, with average Pred/Obs ratio of 1.14; CALPUFF results show significant overpredictions, with Pred/Obs > 3
Portland Model-to-Monitor Comparisons

Table 2. Comparisons of daily maximum 1-hour SO\textsubscript{2} AERMOD and CALPUFF modeled concentrations (ug/m\textsuperscript{3}) based on 100% load and 70% allowable emissions vs. Columbia monitored concentrations.

<table>
<thead>
<tr>
<th>Daily Max 1-hr Rank</th>
<th>Columbia Obs Conc (ug/m\textsuperscript{3})</th>
<th>AERMOD All Adj (ug/m\textsuperscript{3})</th>
<th>AERMOD Pred/Obs All Adj</th>
<th>CALPUFF 1992-93 Met Data (ug/m\textsuperscript{3})</th>
<th>CALPUFF Pred/Obs 1992-93</th>
<th>CALPUFF 2002 Met Data (ug/m\textsuperscript{3})</th>
<th>CALPUFF Pred/Obs 2002</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>479</td>
<td>782</td>
<td>1.633</td>
<td>1335</td>
<td>2.788</td>
<td>2406</td>
<td>5.027</td>
</tr>
<tr>
<td>2</td>
<td>426</td>
<td>531</td>
<td>1.245</td>
<td>1275</td>
<td>2.990</td>
<td>1841</td>
<td>4.317</td>
</tr>
<tr>
<td>3</td>
<td>413</td>
<td>433</td>
<td>1.047</td>
<td>1161</td>
<td>2.808</td>
<td>1759</td>
<td>4.256</td>
</tr>
<tr>
<td>4</td>
<td>356</td>
<td>416</td>
<td>1.169</td>
<td>1127</td>
<td>3.168</td>
<td>1331</td>
<td>3.741</td>
</tr>
<tr>
<td>5</td>
<td>348</td>
<td>356</td>
<td>1.023</td>
<td>1115</td>
<td>3.203</td>
<td>1305</td>
<td>3.751</td>
</tr>
<tr>
<td>6</td>
<td>327</td>
<td>351</td>
<td>1.073</td>
<td>1105</td>
<td>3.380</td>
<td>1100</td>
<td>3.363</td>
</tr>
<tr>
<td>7</td>
<td>306</td>
<td>309</td>
<td>1.010</td>
<td>1057</td>
<td>3.454</td>
<td>1070</td>
<td>3.497</td>
</tr>
<tr>
<td>8</td>
<td>290</td>
<td>301</td>
<td>1.038</td>
<td>1056</td>
<td>3.637</td>
<td>1048</td>
<td>3.609</td>
</tr>
<tr>
<td>9</td>
<td>283</td>
<td>299</td>
<td>1.059</td>
<td>1032</td>
<td>3.654</td>
<td>1015</td>
<td>3.593</td>
</tr>
<tr>
<td>10</td>
<td>277</td>
<td>296</td>
<td>1.068</td>
<td>973</td>
<td>3.508</td>
<td>973</td>
<td>3.509</td>
</tr>
<tr>
<td>Ave</td>
<td>350.5</td>
<td>407.4</td>
<td>1.136</td>
<td>1123.5</td>
<td>3.259</td>
<td>1384.8</td>
<td>3.866</td>
</tr>
</tbody>
</table>
Conclusions

• CALPUFF validation results submitted by NJDEP show generally good performance, similar to AERMOD performance for MCR but not clearly superior
• CALPUFF performance degrades when PRIME downwash is included and when AMS8 monitor is excluded
• Model-to-monitor comparisons for new Columbia monitor show much better agreement based on AERMOD, with CALPUFF showing significant overprediction; these relative differences are similar to differences in AERMOD vs. CALPUFF results submitted with NJDEP 126 petition