Evaluation of LRT Models to Estimate Single Source Impacts on Secondary Pollutants as Part of the IWAQM Phase 3 Process

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Midwest/Central States Air Quality Workshop
April 23, 2014

Outline

- Overview of the IWAQM Process
- Introduction on long range transport (LRT) models and their role in regulatory air modeling
- Background on EPA evaluation program
  - Evaluation paradigm
  - Statistical frameworks
  - Candidate model platforma
- Review of results from

Interagency Workgroup on Air Quality Modeling (IWAQM)

- Originally formed in 1991 to provide a focus for development of technically sound regional air quality models for regulatory assessments of pollutant source impacts on Federal Class I areas
- Participating Federal agencies: the Environmental Protection Agency (EPA), the U.S. Forest Service (USFS), the U.S. Fish and Wildlife Service (USFWS), and the National Park Service (NPS)
- The original purpose was to review respective modeling programs, develop an organizational framework, and formulate reasonable objectives and plans that could be presented to management for support and commitment.

Interagency Workgroup on Air Quality Modeling (IWAQM)

- The IWAQM process largely concluded in 1998 with the publication of the Interagency Workgroup on Air Quality Modeling (IWAQM) Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts (EPA-454/R-98-019).
- The IWAQM Phase 2 report provided a series of recommendations concerning the application of the CALPUFF model for use in regulatory long range transport (LRT) modeling.
- Draft updates to the IWAQM Phase 2 report were released in 2009 to better reflect the state-of-the-practice of long range transport (LRT) modeling techniques.

IWAQM Phase III

- EPA granted Sierra Club petition with commitment to update Appendix W to address O_3 and secondary $PM_{2.5}$ impacts
- Comments received from the 10th Modeling Conference (March 2012) from stakeholders support this interagency and within-agency collaboration effort
  - comments also support the idea of this collaborative effort working in parallel with stakeholders to further model development and evaluation.
- The purpose here is to inform EPA's commitment to update Appendix W, as appropriate, to address chemically reactive pollutants in near field and long range transport applications.

IWAQM Phase III

- This phase will consist of 2 separate working groups, one focused on long-range transport of primary and secondary pollutants and the other on near-field single source impacts of secondary pollutants.
- In addition to the focused work groups, a steering committee will be established to more broadly coordinate across Federal partners and stakeholders

The Primary Objectives of Phase 3

- Identify appropriate air quality models or modeling technique(s), which may include reduced form models for primary and secondarily formed air pollutants under various transport conditions for use in PSD increment and NAAQS compliance analyses;
- Identify the process and methods for model/technique evaluation, the criteria by which the performance those modeling techniques shall be evaluated, and optionally provide example performance evaluations;
- Identify evaluation databases and existing evaluations and how these results will be used to support model performance evaluation and as appropriate model improvement;
- Ensure that all air quality models or modeling techniques and computer codes deemed acceptable by the IWAQM are peer reviewed, publicly available, and fully documented including user guides and other necessary guidance;
- Develop and update guidance documents and revisions to Appendix W where appropriate

Next Steps

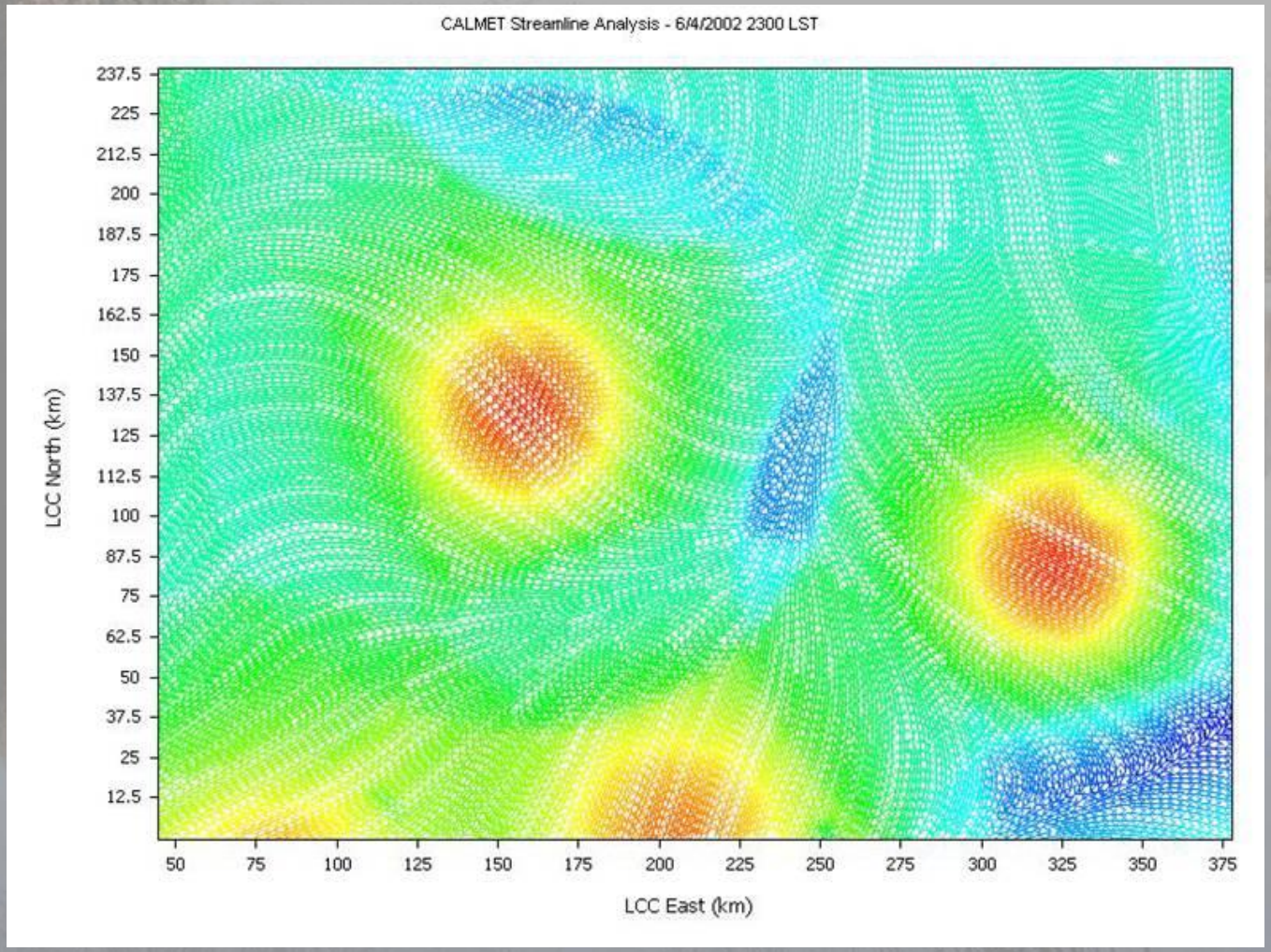
- Currently organizing participants for the work groups and steering committee
- Once these preliminary groups have been established, opportunities will be pursued to engage with stakeholders including State/Local agencies and Tribes

Example - Issues We Have Tackled

- KDHE conducted initial screening of their list of BART eligible sources and notified sources of results. CENRAP's NOOBS CALMET dataset used for initial screening process. Sources shown to be significant were given the option to conduct "refined" screening analyses by the incorporation of observations.

- Initial comparison between results from NOOBS and "refined" screening yielded significant differences. In some instances, NOOBS screening showed very high visibility impacts as compared to no visibility impacts with the incorporation of observations on a number of days. This suggested significant differences in the wind fields between the two methods used to construct wind fields.

The End Result…



The Current State of Practice - IWAQM Phase 2 Revisited

- Ease of use and data availability can breed complacency
  - No statistical evaluation of either prognostic or diagnostic meteorological fields as required under Appendix W, Section 8.3(d)
  - No or minimal visualization of diagnostic meteorological fields deemed critical under IWAQM Phase 2 guidance.
- EPA initially responded in May 2009
  - “The required expertise and collective body of knowledge in mesoscale meteorological models has never fully emerged from within the dispersion modeling community to support the necessary expert judgment on selection of CALMET model control options.”
  - “The lack of a sufficient body of knowledge with respect to mesoscale meteorological models, model evaluation procedures, and related issues has resulted in a process whereby the dispersion modeling community typically obtains the most readily available numerical weather prediction (NWP) dataset for applications of CALMET/CALPUFF without regard to its suitability, creates a three year CALMET dataset, and performs no additional assessment of the resulting CALMET meteorological fields. “

…And Then the Lockdown is Enforced

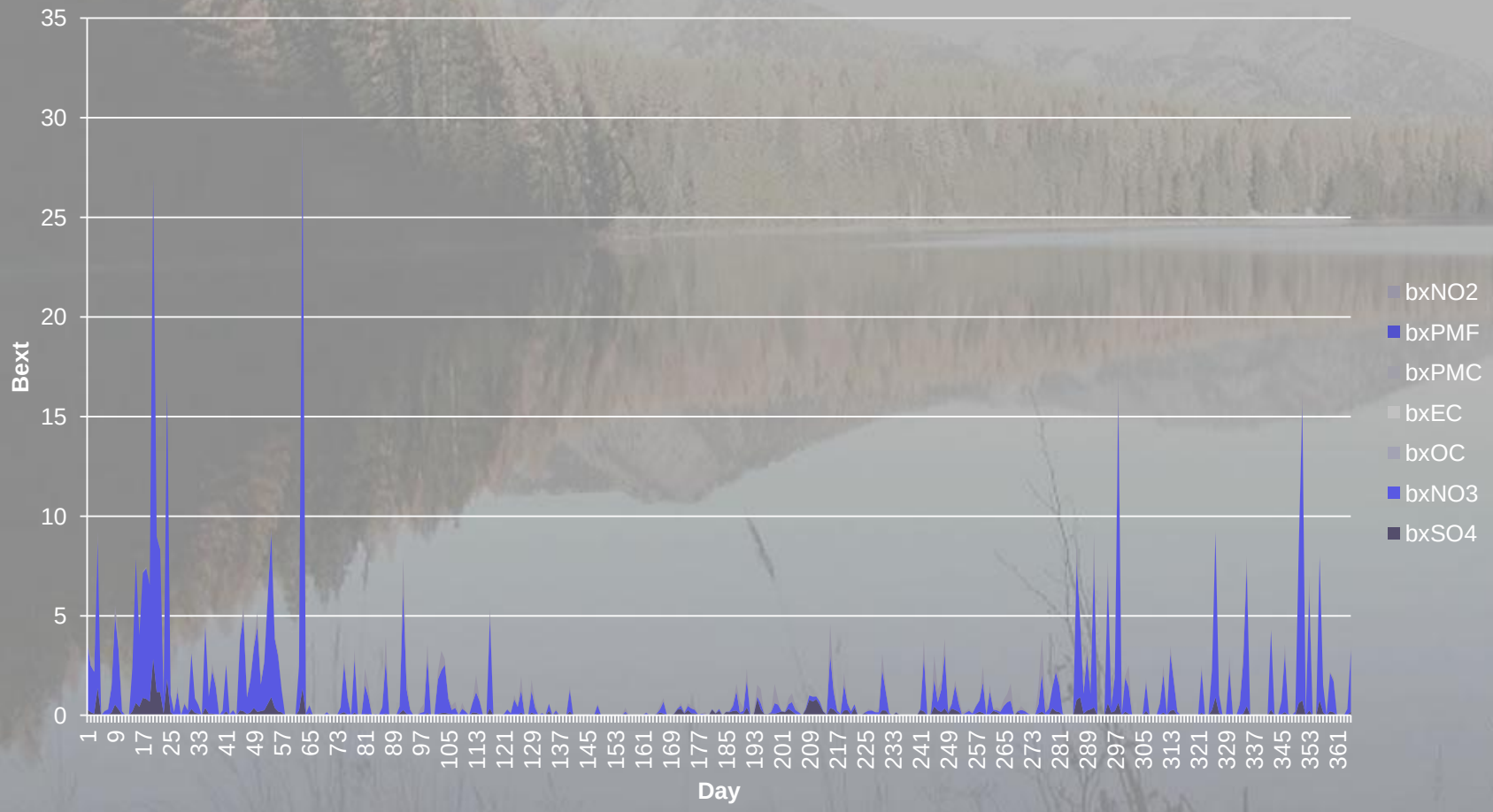
"*The situation described above and public comments have compelled the EPA to reassess the existing guidance and standard practices for the application of CALMET. Whereas in the past it was deemed to be both 'premature and counter-productive' to recommend specific CALMET model control options, the EPA now believes it is both timely and necessary to specify such items to promote scientific integrity and restore balance to the public decision making process.*"

- Interim recommendations from May 2009 were intended to configure CALMET as a pass through, to preserve as much of the integrity of the prognostic meteorological fields
- EPA issues Model Clearinghouse memorandum in August 2009 identifying 'preferred' CALMET model control options. Final model control options based upon EPA/FLM statistical performance evaluations.

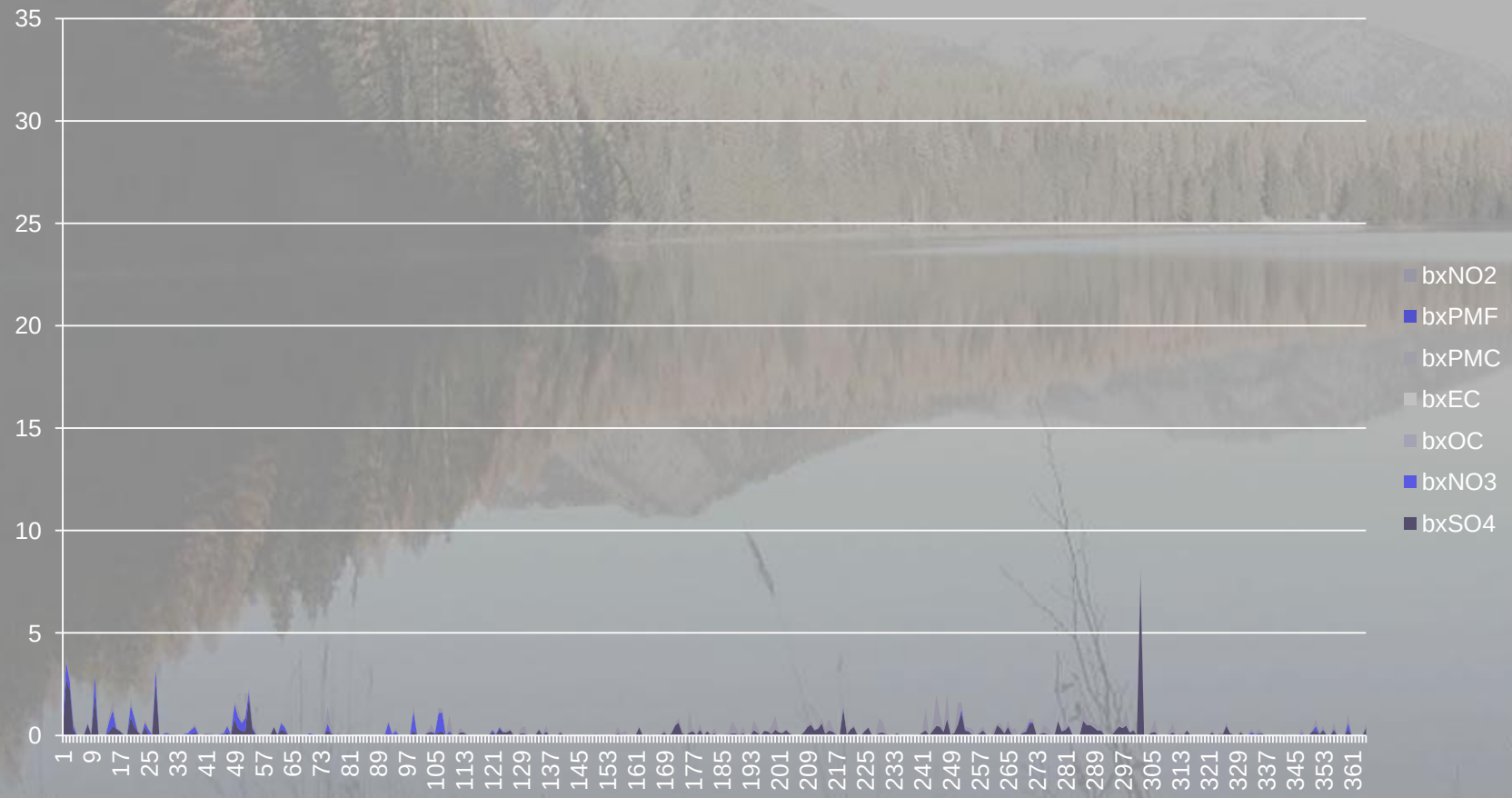
Model Version Issues

- The lack of specificity in the BART guidelines in modeling led to the use multiple of versions of the CALPUFF modeling system. Prior to June 2007, we saw no less than 4 different versions of the CALPUFF modeling system being employed
  - 5.711a, 5.756, 6.112, and 6.221
- In 2010, a new version introduced substantive modifications to the CALPUFF chemical mechanism (versions 6.34 and 6.42) which fundamentally altered the model predictions and virtually eliminated source impacts compared to the EPA approved version (5.8). The updated model was used by large EGUs in BART determinations in Colorado, New Mexico, Arizona, and Nevada.

Simulated Extinction Budget (MEVE1) - CALPUFF v5.8 - MESOPUFF-II, No Ammonia Limiting, 4-KM CALMET



Simulated Extinction Budget (MEVE1) - CALPUFF v6.42 - RIVAD/ISOROPPIA, RADM Aqueous, No Ammonia Limiting, 4-KM MMIF



HISTORICAL USEPA LRT MODEL EVALUATION EFFORTS

Evaluation Efforts at a Glance

- 1986 8-model study
- 1990 Rocky Mountain Acid Deposition Model Assessment Program
- 1993 Interagency Workgroup on Air Quality Modeling Phase I Evaluation
- 1998 Interagency Workgroup on Air Quality Modeling Phase II Evaluation

1986 USEPA Short-Term Long Range Transport Model Evaluation Project

- Eight long range transport models evaluated in the project for consideration as Appendix A LRT model:
  - MESOPUFF (Environmental Research and Technology, Inc.)
  - MESOPLUME (Environmental Research and Technology, Inc.)
  - MSPUFF (ND Dept. of Health)
  - MESOPUFF II (Environmental Research and Technology, Inc.)
  - MTDDIS (Rockwell International, Inc.)
  - ARRPA (Tennessee Valley Authority)
  - RADM (Dames and Moore, Inc.)
  - RTM-II (Systems Applications, Inc.)

- Models Evaluated Across Multiple Data Organization Strategies
  - Space/Time Paired
  - Paired in Space
  - Unpaired in Time
  - Unpaired in Space/Time, etc.

Rocky Mountain Acid Deposition Model Assessment Project

- Acid Rain Mountain Mesoscale Model (ARM3) (SAI) developed for Western Acid Deposition Task Force.
- Compared against 7 other models from 1986 LRT study
  - Evaluated using same approach as 1986
    - Oklahoma and SRL data sets
    - AMS statistics for various data pairing strategies
    - Model scoring system weighted each tracer experiment and data pairing combination equally. Best performing model in each tracer/data combination awarded four points, three points for second, two for third, etc.
      - MESOPUFF-II performed best for unpaired data combination for each tracer experiment
      - ARM3 performed best for both tracer experiments for space/time data pairing.
      - Final overall scoring: ARM3 – 21, MESOPUFF II - 20
  - Model evaluation approach exposes fundamental issue – need for defining performance objectives according to nature of regulatory applications and defining an objective scoring scheme reflecting these performance objectives.

Interagency Workgroup on Air Quality Modeling (IWAQM)

- Phase I Evaluation – “off-the-shelf” models, ARM3 and MESOPUFF-II evaluated, coding errors discovered in ARM3, leaving MESOPUFF II only model available
- Phase II Evaluation – CALPUFF/CALMET and CITPUFF/NUATMOS evaluated.
  - Trajectory evaluation using CALMET and NUATMOS using observations and “hybrid” fields based upon observation blending with 80-km MM4 data.
  - Statistical evaluation using ASTM/Irwin methods for evaluation (Oklahoma and SRL datasets).
    - CALMET/MM4 combination produced more accurate trajectory statistics than NUATMOS/MM4 combination

Lessons Learned from Prior Evaluation Efforts

- No USEPA recommended methodology for evaluation of air quality models. No consistent approach between efforts in 1980's and 1990's.
- Evaluation methodology used all published AMS metrics and data organizational strategies. This did not take into consideration regulatory use of LRT models, weighting schemes not most appropriate for particular methods LRT models are used for.
- High sensitivity of LRT models to meteorological inputs. Need for more objective meteorological performance evaluation measures.
- No data sets available to evaluation chemical transformation mechanisms of LRT models

Paradigm Question

- Carhart et al. (1989) noted that there was no recommended USEPA modeling guidance specific LRT models. 1986 EPA study applied all model metrics across all data organization strategies in the evaluation of the 8 models included in that study.
  - Are LRT models dispersion models or chemistry models?
    - Concerned about peak values
    - Concerned about accuracy of transport
    - Concerned about transformation and removal mechanisms
- Should they be evaluated in the same manner as near-field dispersion models, photochemical grid models, or some other way?

1984 USEPA Interim Evaluation Procedures Document

- The USEPA interim procedures document suggests:
  - definition of performance objectives relative to the nature of the regulatory applications of the model;
  - compilation of data sets and performance measures that will be used for each performance objective;
  - objective scheme for assigning weights to each performance measure and data set combination; and
  - an objective scheme for scoring the performance of any models relative to one another.

Defining Performance Objectives – Start with Regulatory Use of Model

- Current Regulatory Uses:
  - PSD Class I NAAQS and increment analyses
  - Visibility and deposition for Air Quality Related Values analysis for PSD
- Future Uses:
  - Single source O_3 NAAQS analyses
  - Single source $PM_{2.5}$ NAAQS analyses

Regulatory Niche for LRT Models

- Section 165(d) of the Clean Air Act requires suspected adverse impacts on federally protected Class I areas be determined under the federal major new source review program called Prevention of Significant Deterioration of Air Quality (PSD) program
- Many Class I areas are located areas are located more than 50 km from source under review.
- EPA near field regulatory models (ISC, AERMOD, etc.) not applicable beyond 50 km because steady-state wind field assumption not applicable beyond these distances
- LRT models used to assess PSD increment, visibility impacts from secondary aerosols, and acid deposition in federally protected Class I areas

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Initial EPA Efforts for IWAQM Phase 3

- EPA WA 4-06: Single-Source LRT Model Evaluation (7 Tasks)
  - Task 1: Work Plan
  - Task 2: Update and Finalize MMIF
  - Task 3: CALPUFF Met-Input NetCDF for Visualization
  - Task 4: Document CALPUFF Tracer Test Evaluations
  - Task 5: Critical Review of Single-Source LRT Models
  - Task 6: Proof of Concept for using PGMs for Single-Source AQ/AQRV Assessments and Compare with CALPUFF
  - Task 7: Evaluate LRT Models using Tracer Test and Plume Chemistry Field Experiments

Testing Advection and Diffusion of Models

MESOSCALE TRACER SIMULATIONS

Evaluation Framework

- Evaluation of LRT models within their defined regulatory niche requires an evaluation of three independent components of the AQ model system
  - Meteorological component
  - Advection and diffusion component
  - Chemical transformation

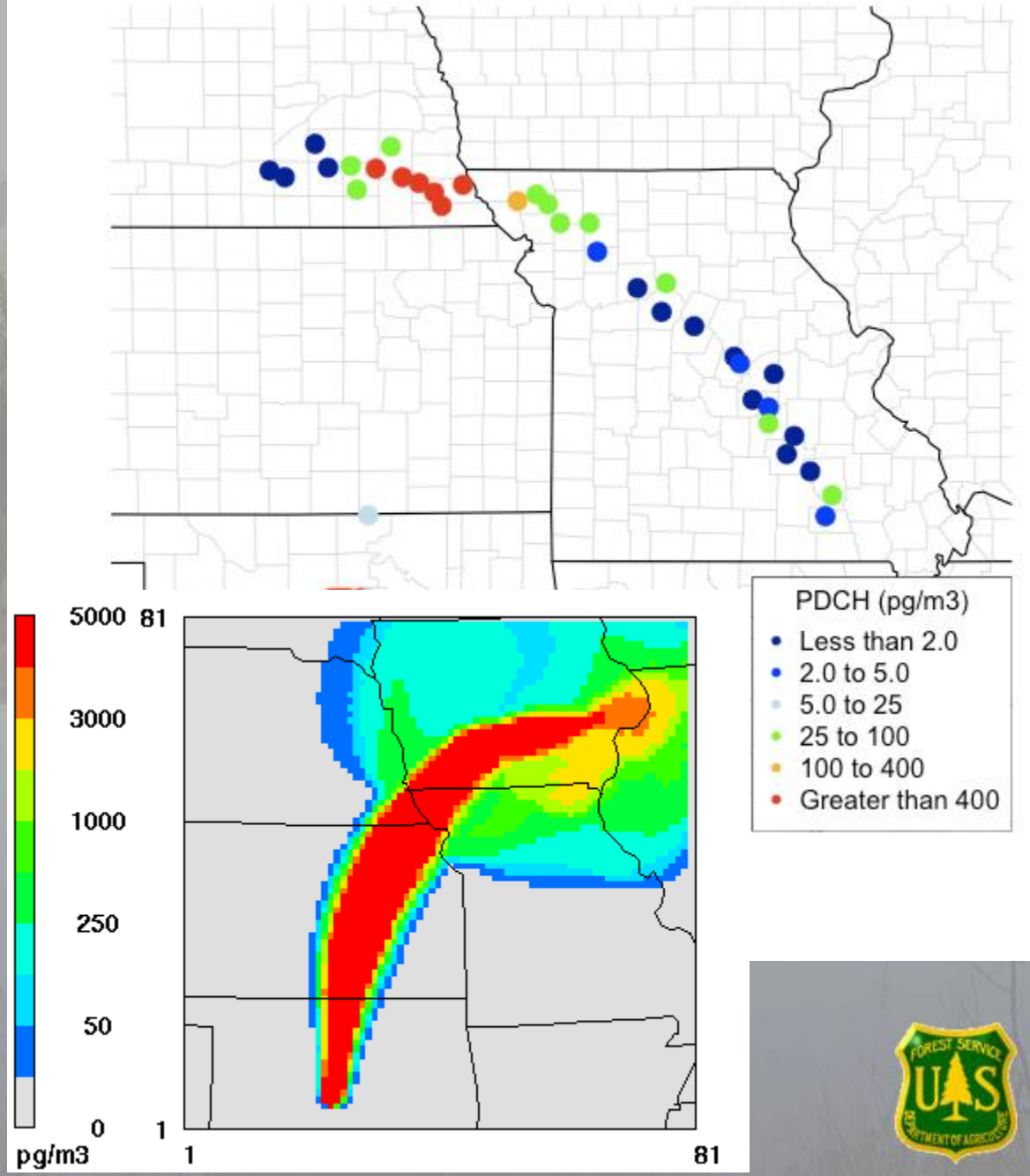
Models Evaluated for Inert Tracers

- Three Distinct Class of Models
  - Lagrangian Puff Models
  - Lagrangian Particle Models
  - Eulerian Grid Models

- CALPUFF Version 5.8 (EPA approved version)
- MM5-FLEXPART (Version 6.2)
- HYSPLIT (Version 4.8)
- SCIPUFF (Version 2.303)
- CAMx (Version 5.20)
- CALGRID (Version 2.4)

Long Range Transport Analysis of Inert Tracer Studies

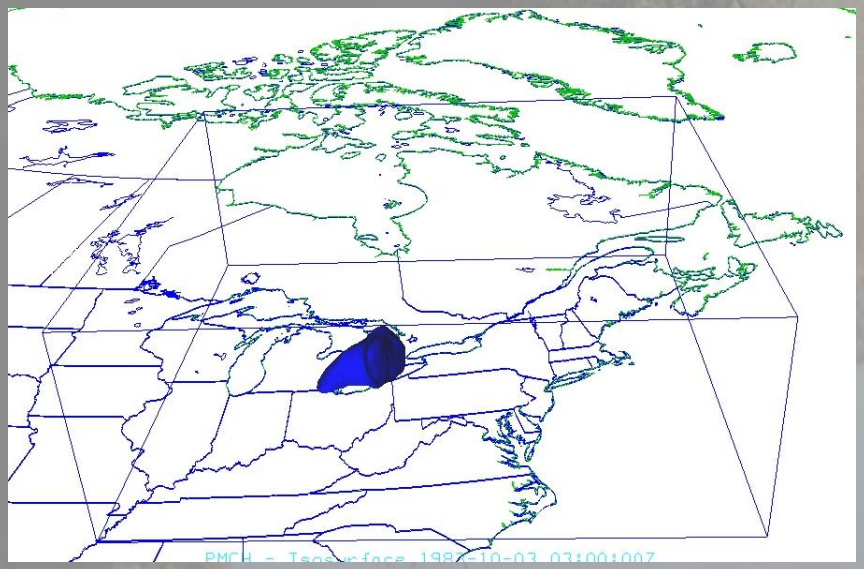
- Designed to examine the advection/diffusion capabilities of models
- Example presented here is CAMx for GP80 experiment on 600-km arc of monitors.

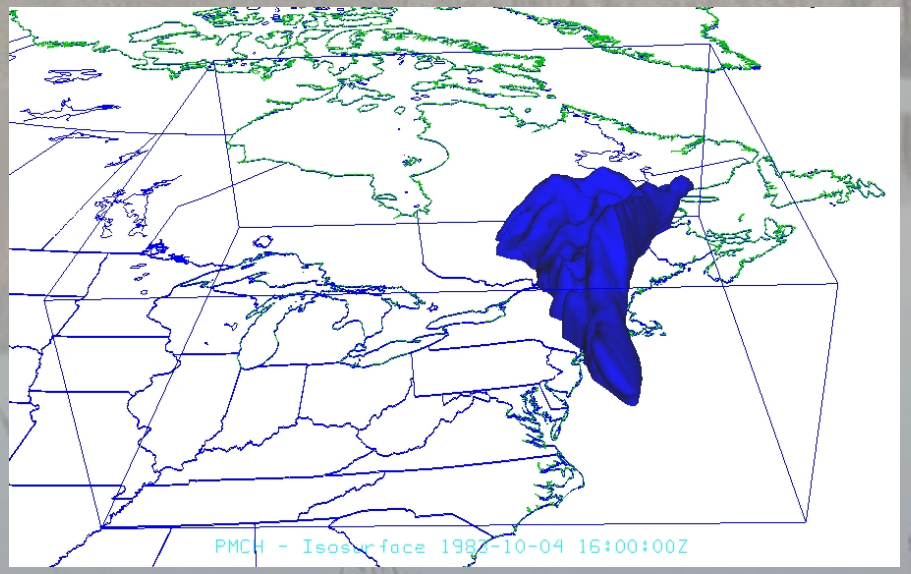


"Documentation of the Evaluation of CALPUFF and Other Long Range Transport Models Using Tracer Field Experiment Data"

http://www.epa.gov/scram001/reports/EPA-454_R-12-003.pdf here is

Example - CAPTEX





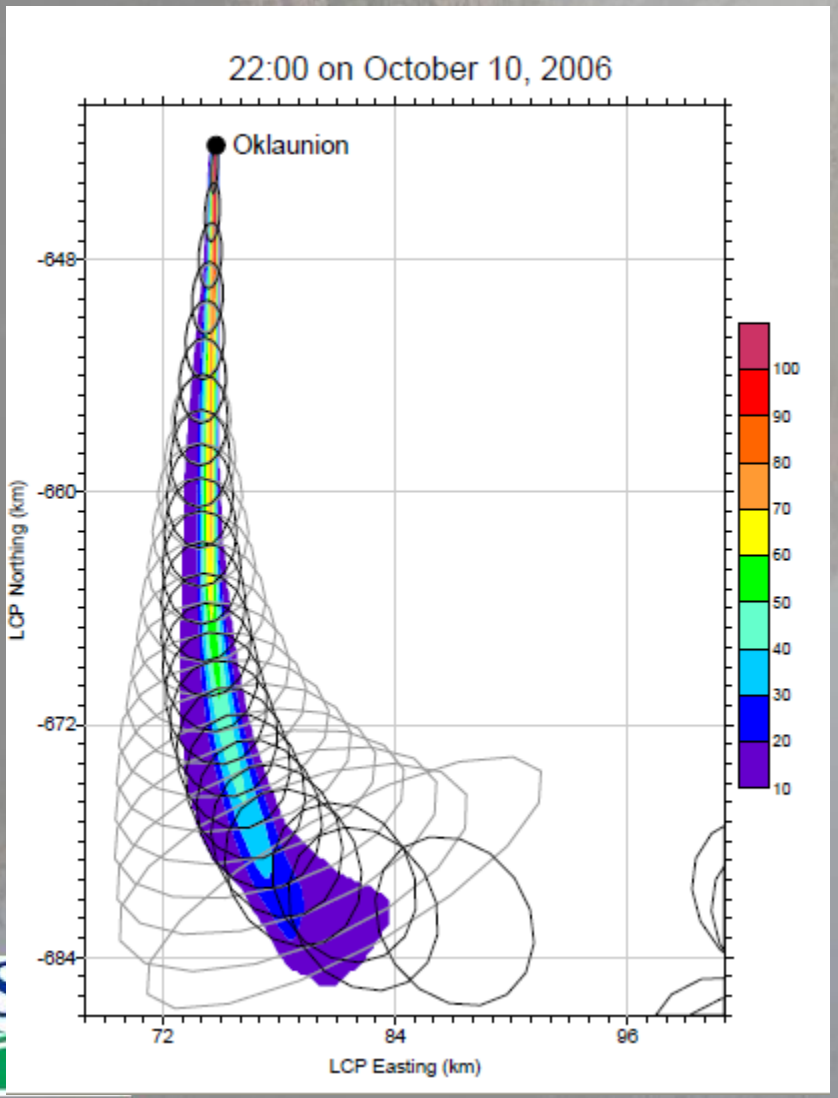
Testing Chemistry of Models

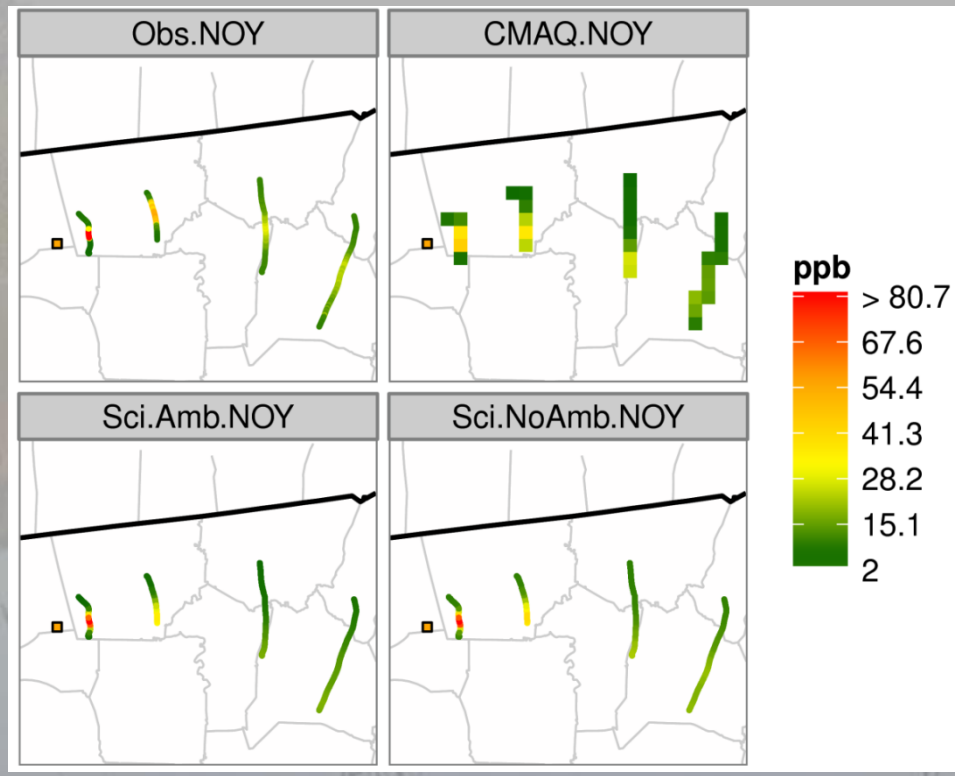
AIRCRAFT OBSERVATION COMPARISONS

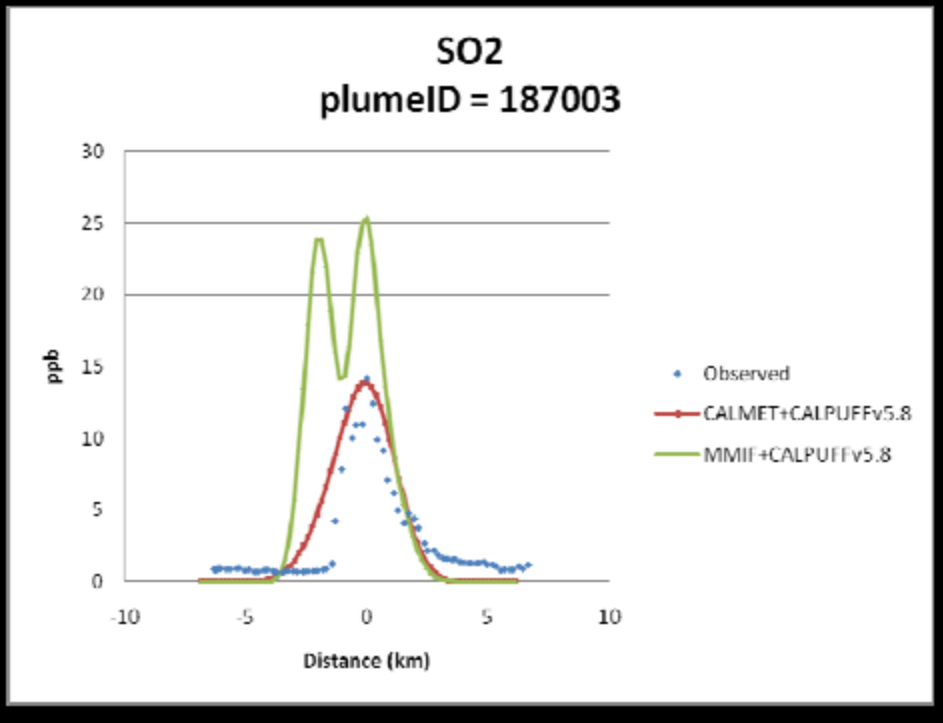
Single Source Chemistry Evaluations

- Application of LRT models for chemistry usually only involve an individual or small group of sources.
- Traditional photochemical grid model (PGM) evaluation techniques (chemistry evalaution) combined with inert tracer evaluation (advection and diffusion) are combined to examine the suitability of a model for use in single source chemistry applications.
  - The best performing chemistry model will only be as good as its ability to treat advection and diffusion appropriately.
- Results of effort documented in ENVIRON report "Evaluation of Chemical Dispersion Models using Atmospheric Plume Measurements from Field Experiments"

CAMx, SCICHEM, and CMAQ Evaluation



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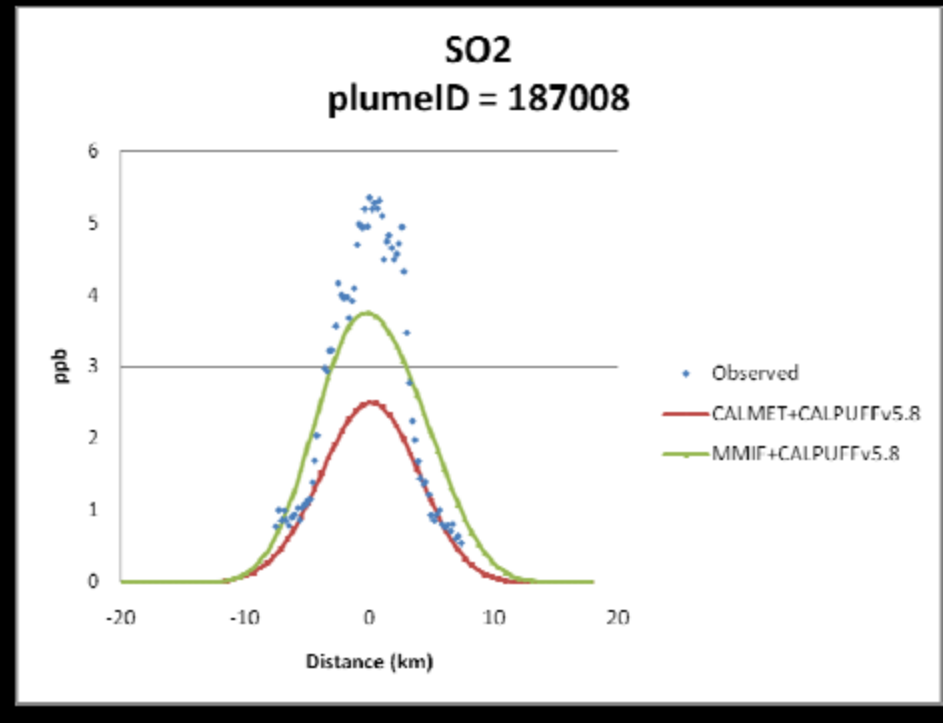
ppb
Distance (km)
Observed
CALMET+CALPUFFv5.8
MMIF+CALPUFFv5.8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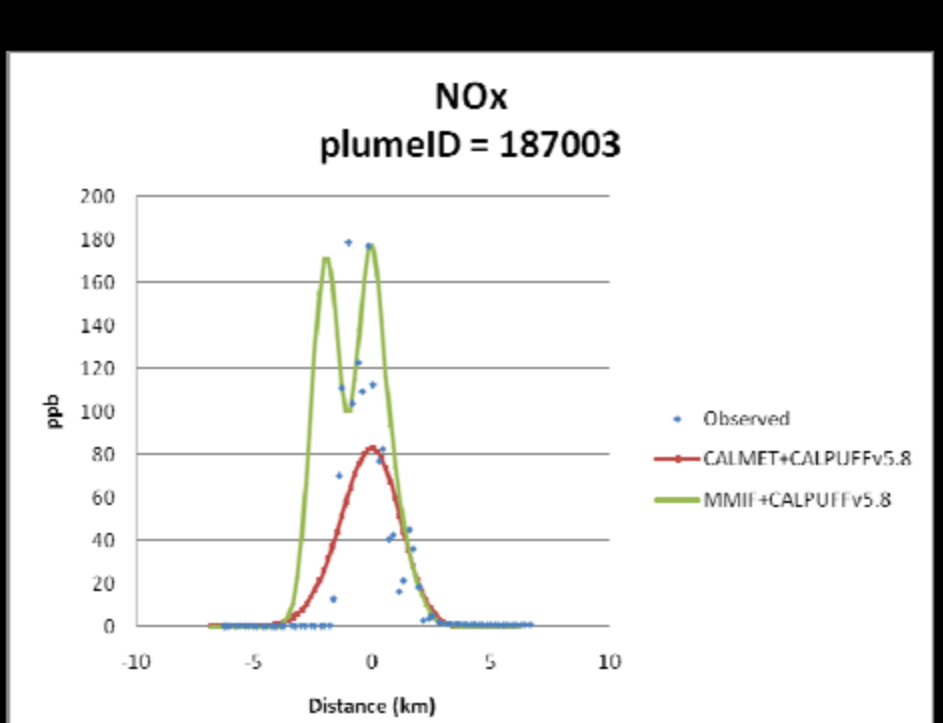
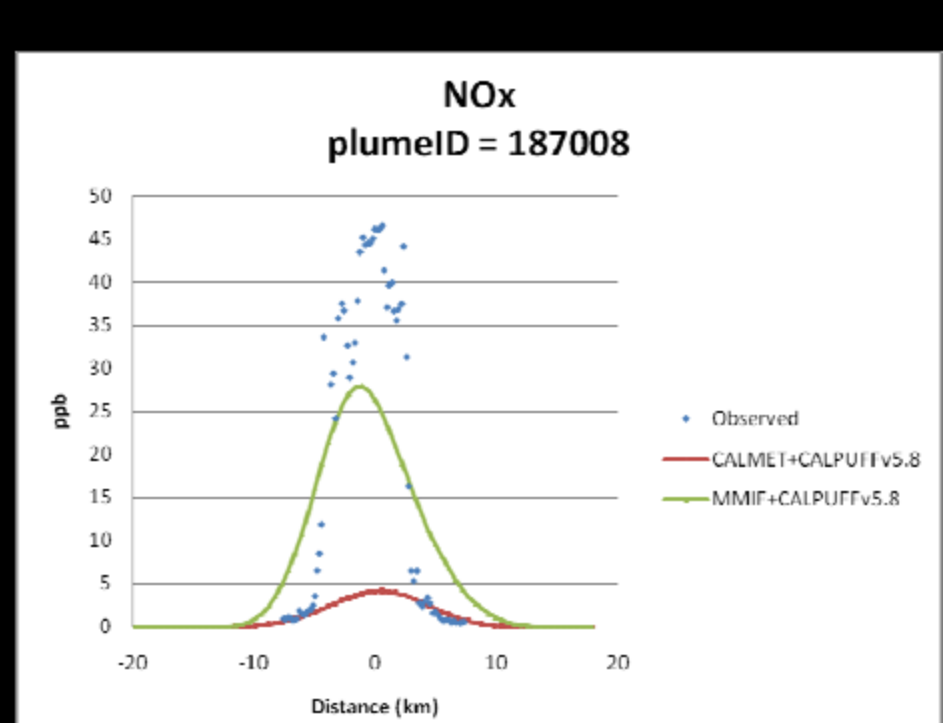
ppb
Distance (km)
Observed
CALMET+CALPUFFv5.8
MMIF+CALPUFFv5.8


NOx
plumeID = 187003
ppb
Distance (km)
Observed
CALMET+CALPUFFv5.8
MMIF+CALPUFFv5.8


NOx
plumeID = 187008
ppb
Distance (km)
Observed
CALMET+CALPUFFv5.8
MMIF+CALPUFFv5.8

What's Next?

- Federal land management agencies want to progress toward better, state-of-the-science models and to promote greater consistency in the application of models in the regulatory process.
  - "Improvements" during regulatory actions are not a good way proceed, but is somewhat of a reality since permits are where modeling is funded

FLM Efforts

- FWS/USFS testing of PGM's for AQRV assessments
  - Building upon EPA study "*Comparison of Single Source Air Quality Assessment Techniques for Ozone, $PM_{2.5}$, other Criteria Pollutants and AQRV's*"
  - Examining source apportionment techniques for single source applications
  - Development of standardized procedures and databases to streamline process
- Evaluation of FLAG procedures for PGM assessments
- Assisting EPA in updating pertinent sections of Appendix W

Conclusions

- We want to make sure we are moving forward in modeling to keep pace with science and EPA efforts
- Needs to be an orderly process where things are evaluated – not ad hoc “improvements”
- Not ultimately wedded to any particular modeling platform
- As modeling technique changes would reevaluate FLAG in that context