Using Photochemical Models to Estimate Single Source Impacts on Secondary Pollution

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Outline

- 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 European Tracer Experiments (others in progress)

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
- Future Demands:
  - Single source O_3 impact analysis
  - Single source $PM_{2.5}$ impact analysis

Regulatory Background

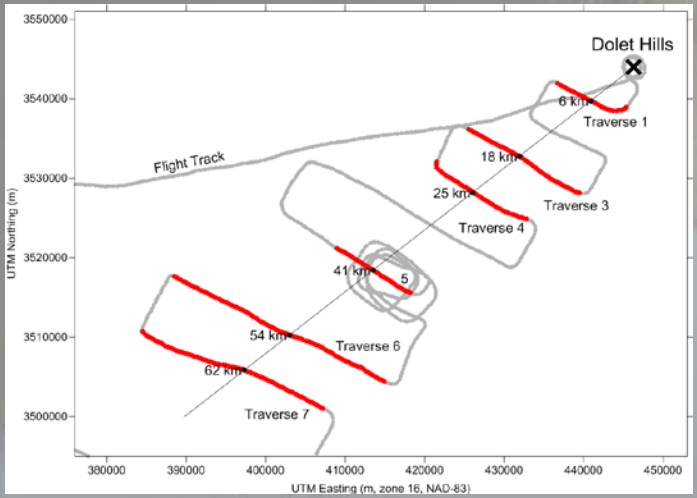
- Interagency Workgroup on Air Quality Models (IWAQM) in 1991 in response to emerging need to assess air pollutant impacts in federal Class I areas.
- In 1998, EPA published IWAQM Phase 2 report recommending CALPUFF for regulatory LRT model applications. Phase 2 report provided recommended settings for CALPUFF model control options.
- In 2003, EPA promulgated the CALPUFF modeling system as its "preferred" model for LRT model applications. IWAQM Phase 2 report becomes de-facto "recommendations for regulatory use" for regulatory CALPUFF applications.
- In 2008-2009, EPA, US Fish and Wildlife Service, National Park Service, and US Forest Service reconvene IWAQM to update Phase 2 guidance. LRT model evaluation program initiated by EPA as part of IWAQM effort.
- IWAQM Phase 3 initiated (2009) – evaluation of possible model platforms for development/adaptation for single source, full photochemistry model applications

2009 LRT Model Evaluation Project Goals

- Develop meteorological and tracer databases for evaluation of long range transport models.
- Develop a consistent and objective method for evaluating long range transport (LRT) models used by the EPA and FLM's.
- Promote the best scientific application of models based upon lessons learned from evaluations and reflect this in EPA modeling guidance.
- Evaluate new models as part of IWAQM Phase 3 process.

EPA LRT Single-Source Model Evaluation Study

- Test MMIF for CALPUFF, AERMOD and SCICHEM
- Finish report documenting LRT tracer test evaluation



- Single-Source PGM LRT Proof of Concept
  - Demonstrate and compare single-source AQ/AQRV for CAMx, CALPUFF/CALMET, CALPUFF/MMIF and SCICHEM
- Plume chemistry evaluation using aircraft data
  - CAMx, SCICHEM, CALPUFF V5.8 & V6.42

Testing Advection and Diffusion of Models

MESOSCALE TRACER SIMULATIONS

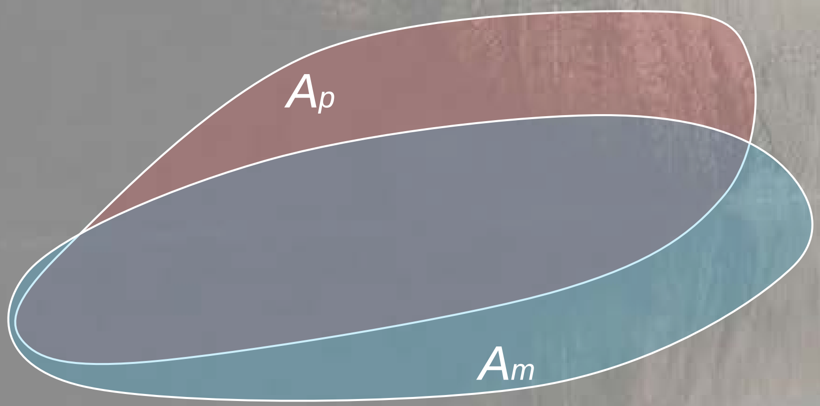
Evaluation Framework

- 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

EPA LRT Tracer Evaluation

- Adopted evaluation approach of ATMES-II experiment (Mosca et al, 1998) as implemented by Draxler et al (2001)
  - NOAA ARL DATEM
    - http://www.arl.noaa.gov/DATEM.php
- Global statistical measures:
  - Scatter (Pearson's Correlation Coefficient, R)
  - Bias (Fractional Bias, FB)
  - Spatial (Figure of Merit in Space, FMS)
  - Cumulative Distribution (Kolomogorov-Smirnov Parameter, KSP)
- Additional spatial performance measures:
  - False Alarm Rate (FAR)
  - Probability of Detection (POD)
  - Threat Scores (TS)
- Temporal analysis
  - Figure of Merit in Time (FMT)
- EPA developing guidance for LRT evaluation
  - Include peak performance measures
  - Also met model evaluation and operational evaluation of chemical mechanism of models

Figure of Merit in Space



$$FMS = \frac{A_M \cap A_P}{A_M \cup A_P}$$

- FMS is defined as the ratio between the intersection of measured (***Am***) and predicted areas (***Ap***) above a significant concentration level and their union. FMS expressed as a percentage corresponding to the degree of overlap.
- The more that the predicted and measured tracer clouds overlap one another, the greater the FMS values are.

Evaluation Paradigm

- Evaluation procedures follow logic of Chang et al (2003) regarding multi-model evaluations
  - Inherent amount of uncertainty due to differences in technical formulations between various modeling systems
  - Use common meteorological platform with minimal diagnostic adjustments to reduce uncertainty
    - This is a challenge when models such as SCIPUFF and CALPUFF use diagnostic wind models as primary source of 3-D meteorological data
      - Use MM5SCIPUFF developed by Penn State and MMIF (CALPUFF) developed by EPA to couple MM5 directly to these models
  - Model control options mostly default “out-of-the-box” configuration
    - CALPUFF configured for turbulence dispersion and puff-splitting similar to SCIPUFF, which is a deviation from its default configuration

Models Under Evaluation

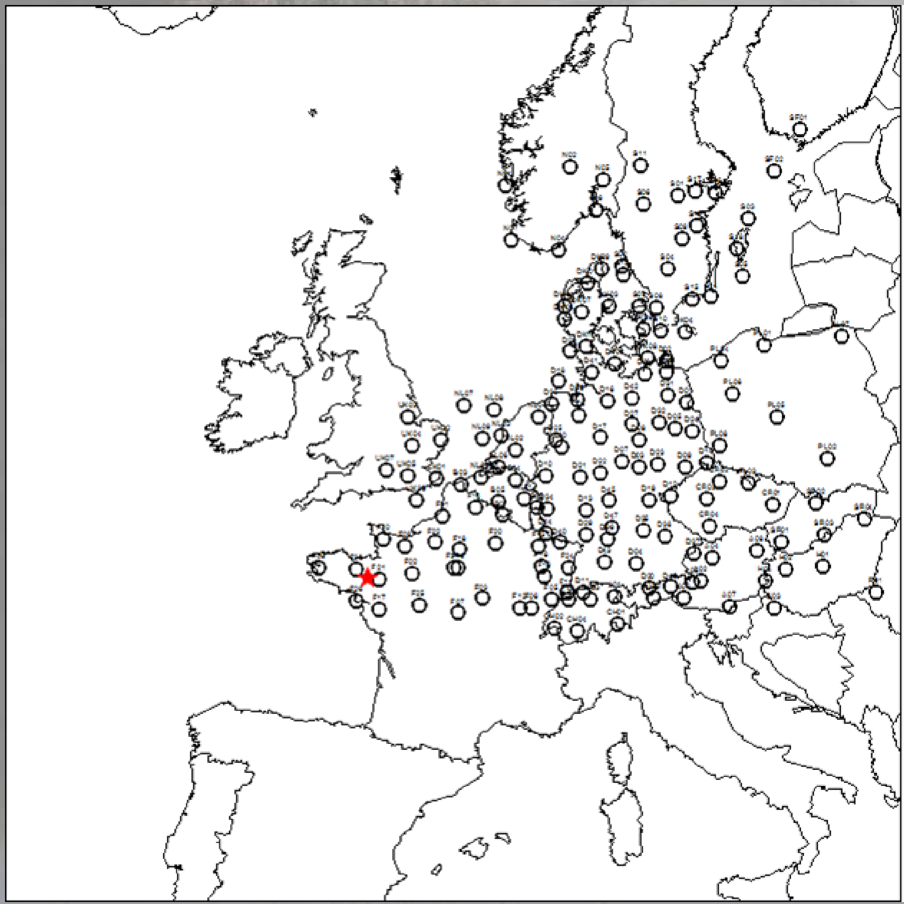
- Three Distinct Class of Models
  - Lagrangian Puff Models
  - Lagrangian Particle Models
  - Eulerian Grid Models

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

CAMx Configuration

- CAMx Version 5.20.1
  - 148 x 112 x 25 (36-km)
  - Inert Tracer, No physical removal
  - OB70, TKE, ACM2, and CMAQ kv
    - OB70, TKE, and ACM2 run with smaller minimum kv than CMAQ option. Potentially leads to differences in dispersive properties among various configurations, especially at night under stable conditions.
    - Current version of OB70 option generates unreasonably low diffusion coefficients relative to other options.
  - BOTT, PPM advection
  - Plume-in-Grid (GREASD)/No Plume-in-Grid
  - Best performance configuration displayed following…

European Tracer Experiment (ETEX)



- ETEX initiated in 1992 by the European Commission (EC), International Atomic Energy Agency (IAEA), and the World Meteorological Organization (WMO) to address many questions that arose from 1986 Chernobyl accident regarding the development of LRT models.
- ETEX was designed to validate LRT models used for emergency response situations and to develop a database which could be used for model evaluation purposes.
- Two perflourocarbon tracer (PFT) releases in October and November 1994.
  - 168 monitoring sites in 17 countries with a samling frequency of 3 hours for 90 hour duration.

ETEX Observed Tracer Pattern

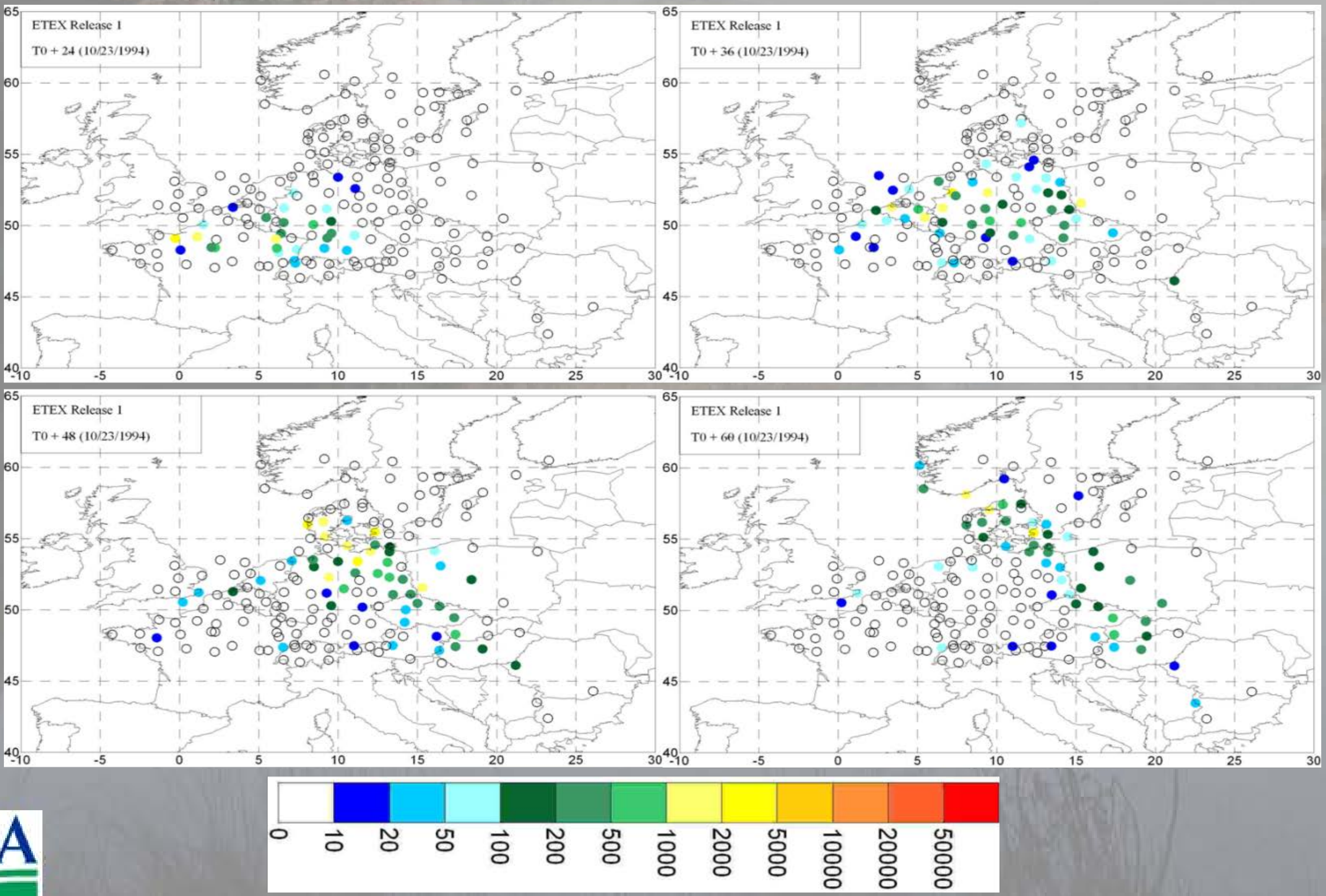
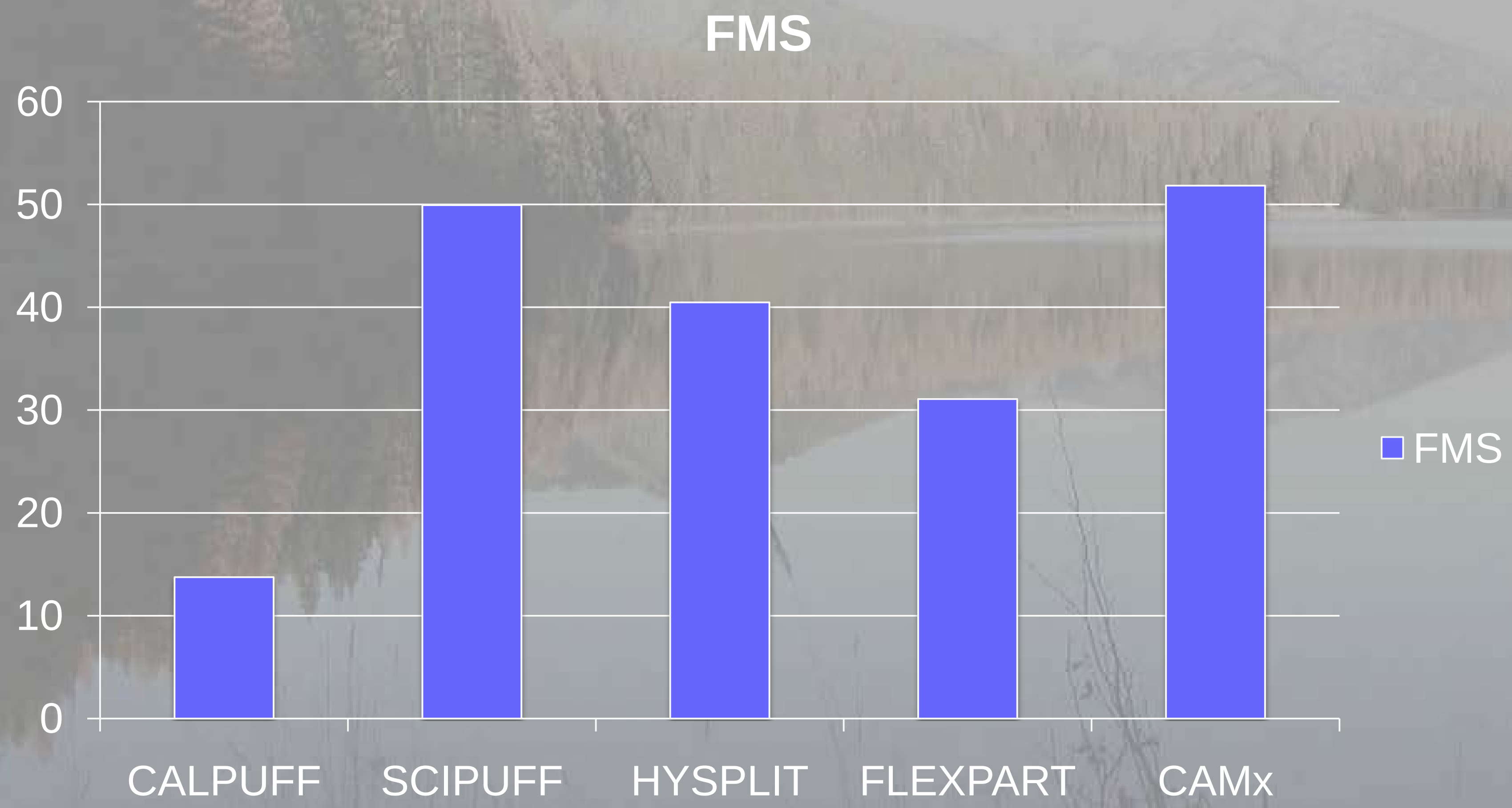
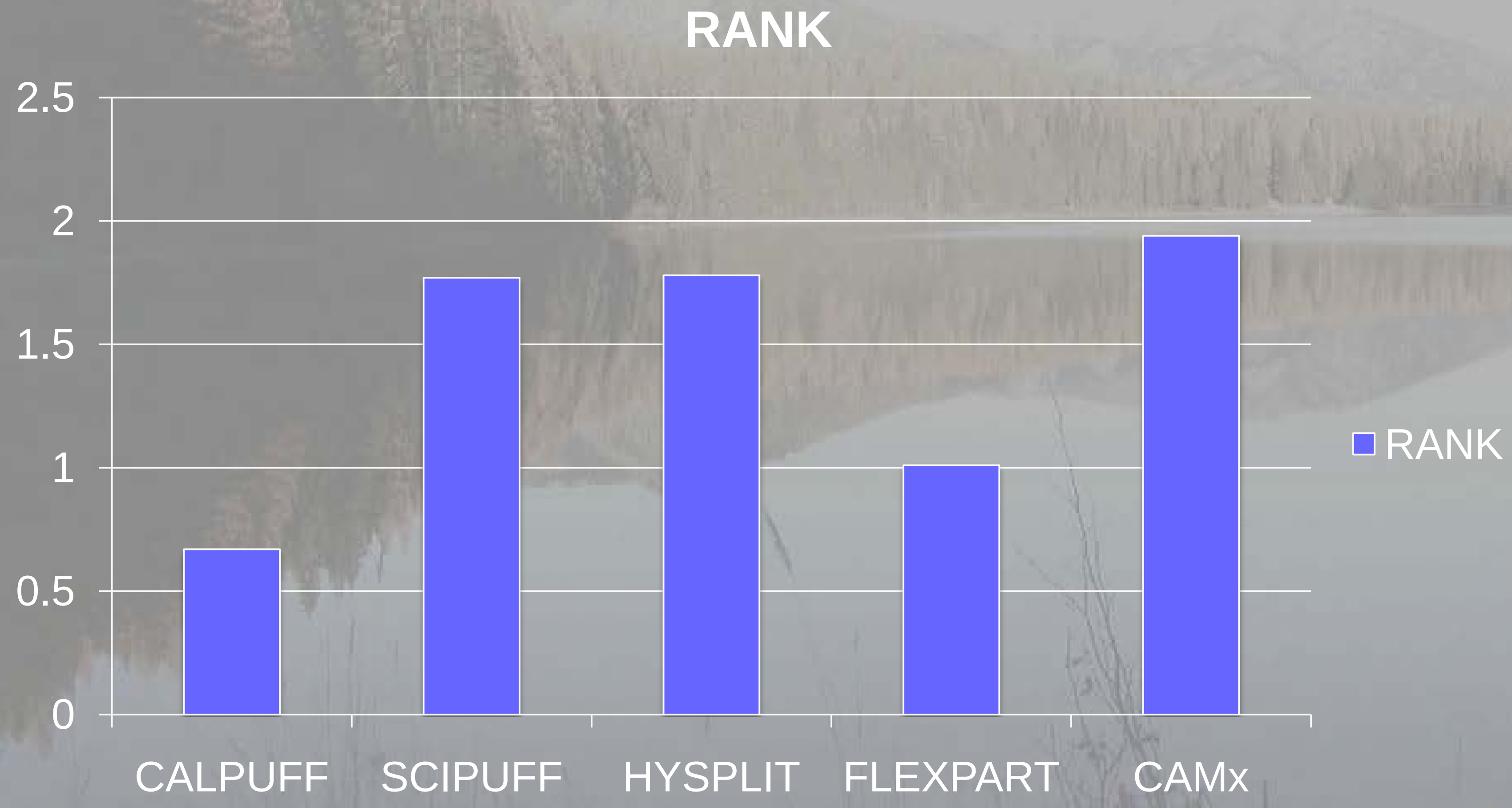


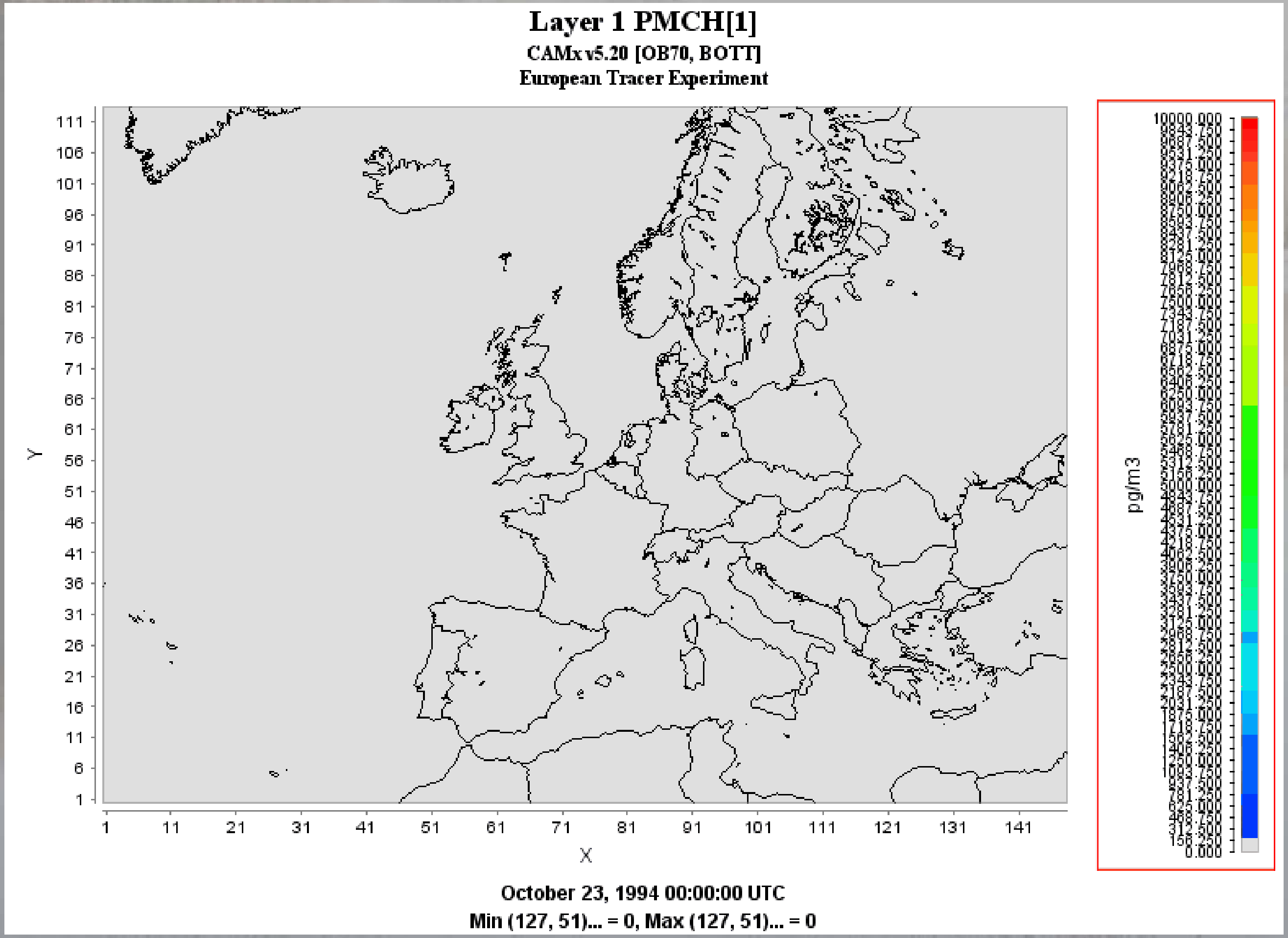
Figure of Merit in Space (Perfect = 100%)



MODEL RANK (PERFECT = 4.0)



ETEX Simulation



Testing PGM’s for BART and PSD Class I AQRV Impacts

PROOF-OF-CONCEPT MODELING FOR PGM’S

Example Visibility Analysis

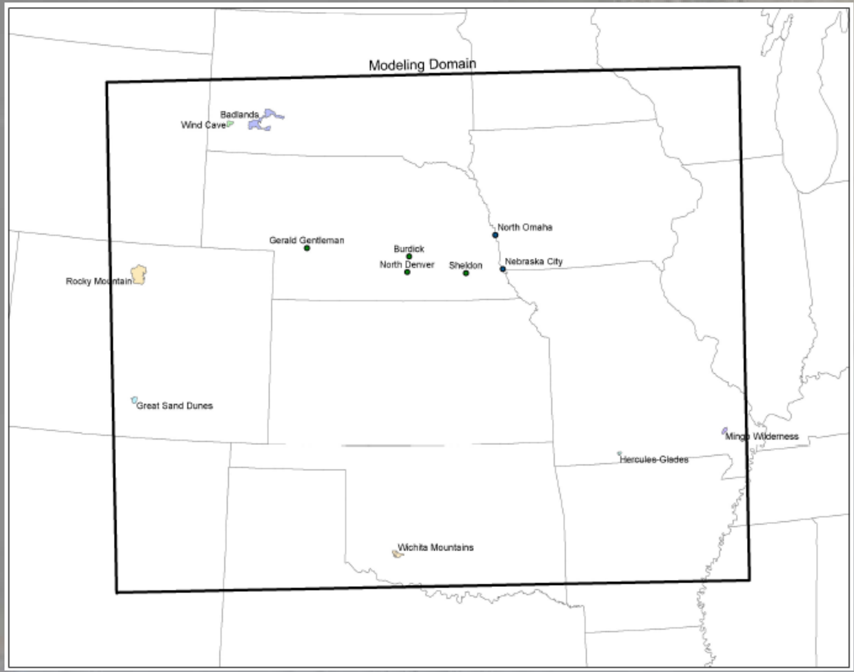
- CALPUFF Version 5.754
  - MESOPUFF II Chemistry
- CALMET Version 5.53a
  - CALMET configured to best preserve original prognostic met
    - Initialized with CENRAP 2002 36-km MM5
    - Prognostic upper air (NOOBS=1)
    - Prognostic precipitation (NPSTA=-1)

- CAMx Version 4.41
  - CENRAP Base02f Inventory
  - CENRAP 36-km MM5 Meteorology
  - Probing Tool: Particulate Source Apportionment (PSAT), Individual source tagging
  - Plume-in-Grid: GREASD PiG
  - Flexinest: Optional 12 km imposed on modeling grid to limit initial dispersion of PiG puffs

Modeling Domains

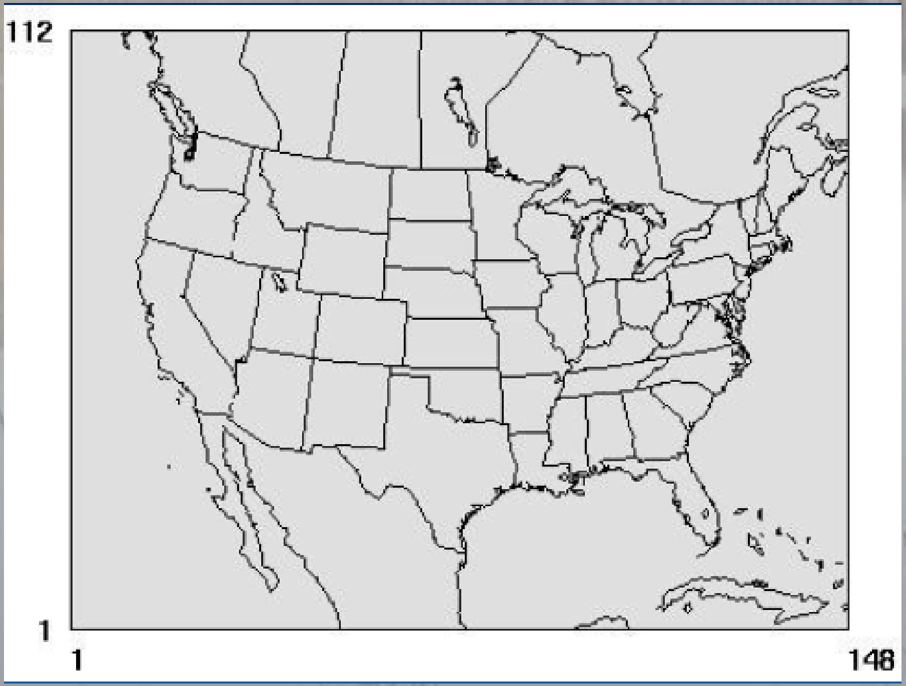
CALPUFF Domain:

243 x 195 x 10 (6-km)

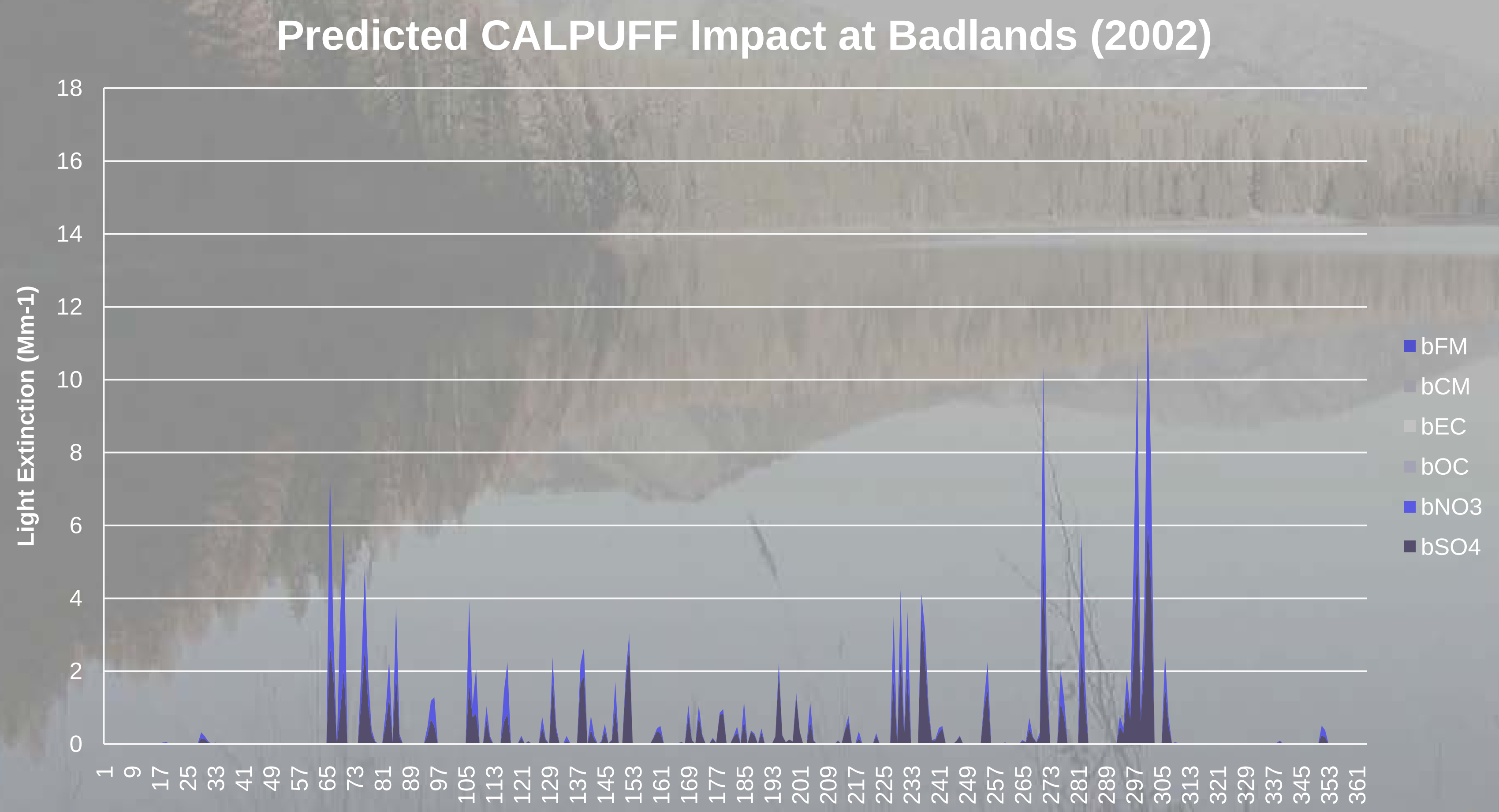


CAMx Domain:

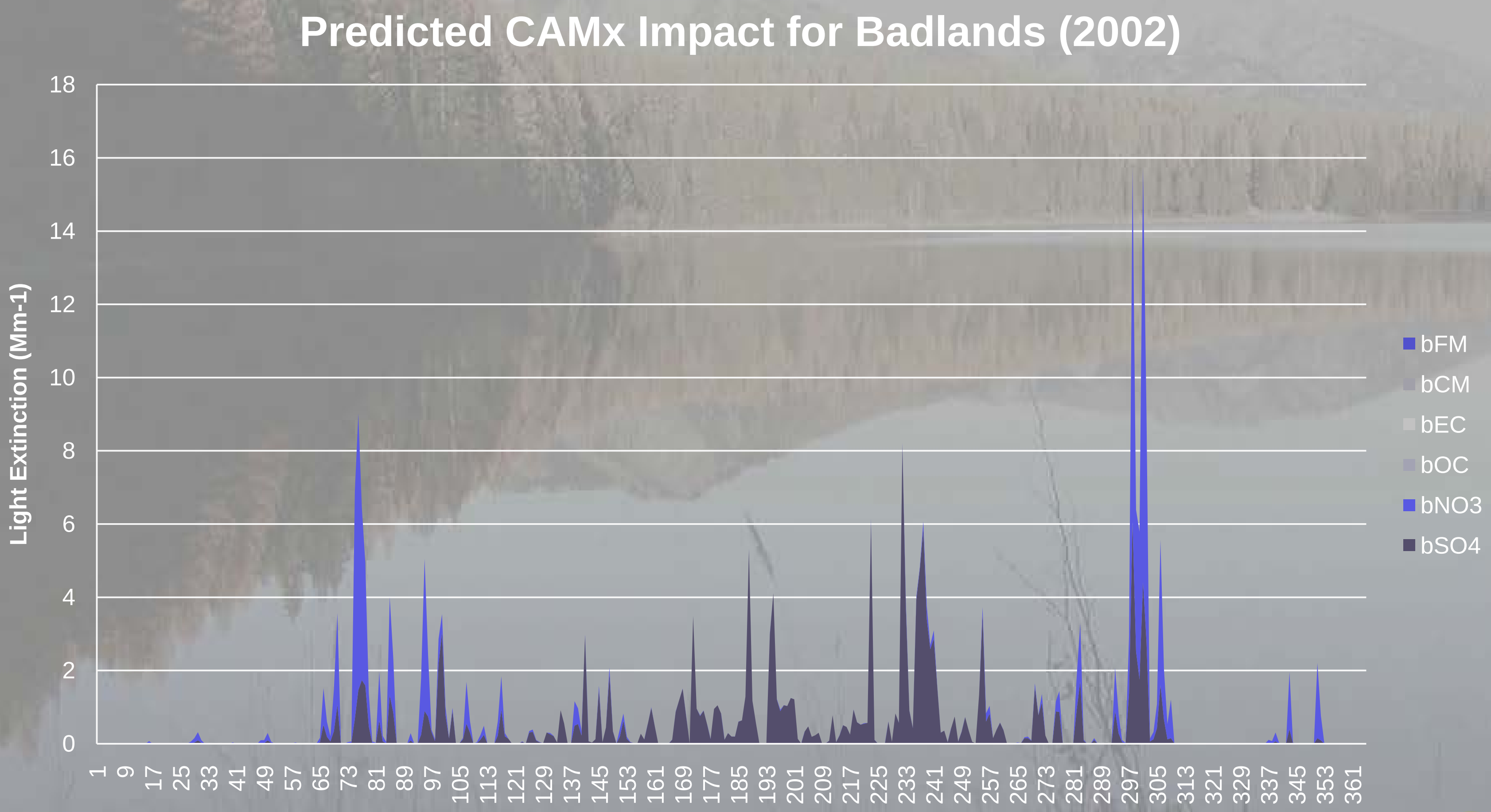
148 x 112 x 19 (36-km)



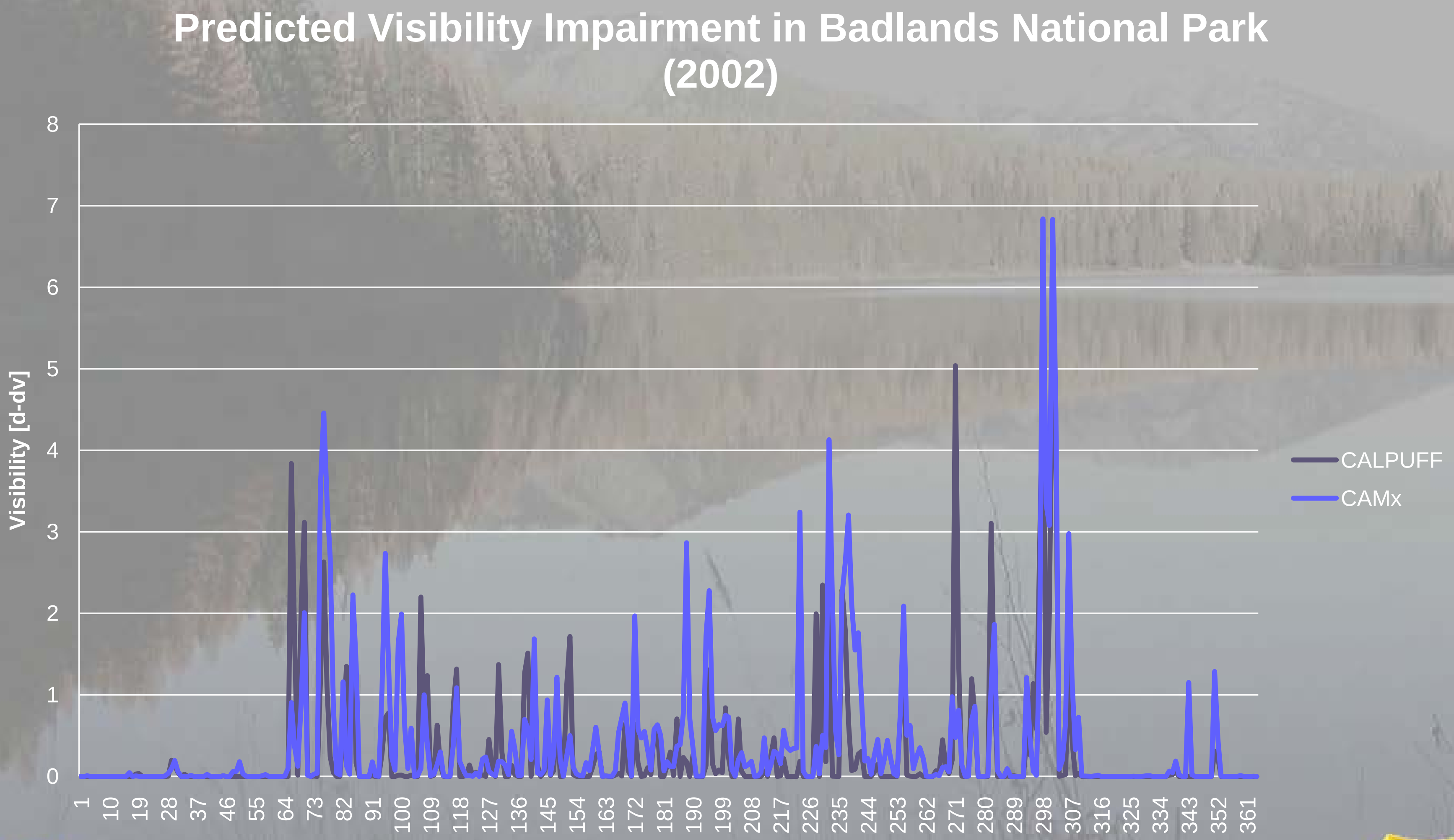
CALPUFF Visibility Impacts



CAMx Visibility Impacts



CALPUFF v. CAMx



SUMMARY AND CONCLUSIONS

Regulatory Considerations

- The differences in the operational paradigms between the two communities will require both the EPA and the FLM's to develop a more rigid set of operational procedures similar to the current permit modeling paradigm in order to insure both a scientifically sound and consistent set of procedures to prevent an 'anything goes' process as would likely develop without such procedures.
  - Static emissions and meteorological databases to insure consistency in application
- EPA will need to evaluate the current PSD and Appendix W regulatory framework
  - PSD requires following Appendix W, so each application of PGM would require Section 3.2 "alternative model" justification for use with both NAAQS and increment demonstrations under current "EPA approved model" architecture.
  - Length of meteorological record for PGM's will likely have to be expanded to be consistent with requirements of GAQM (e.g. 3 years of prognostic data) and to account for interannual variability to capture conditions which drive design value concentrations.
  - Development of significance thresholds for single source (cause or contribute test) required for NAAQS demonstrations (O_3 in particular).

Conclusion

- PGM's capable of assessing single source impacts for both AQRV and ozone requirements under PSD.
- Source apportionment eliminates need for multiple "zero-out" runs
- Significant barriers remain to implementation of PGM's
  - Increased computational requirements
  - Increased training requirements for permit modeling staff
  - Creation of a hybrid regulatory and guidance framework for implementation of PGM's within a regulatory permit modeling paradigm which is highly rigid and prescriptive