8hrC Modeling Update:
Approach & Recent Research Findings

presented to

Southeast Texas Photochemical Modeling Technical Committee

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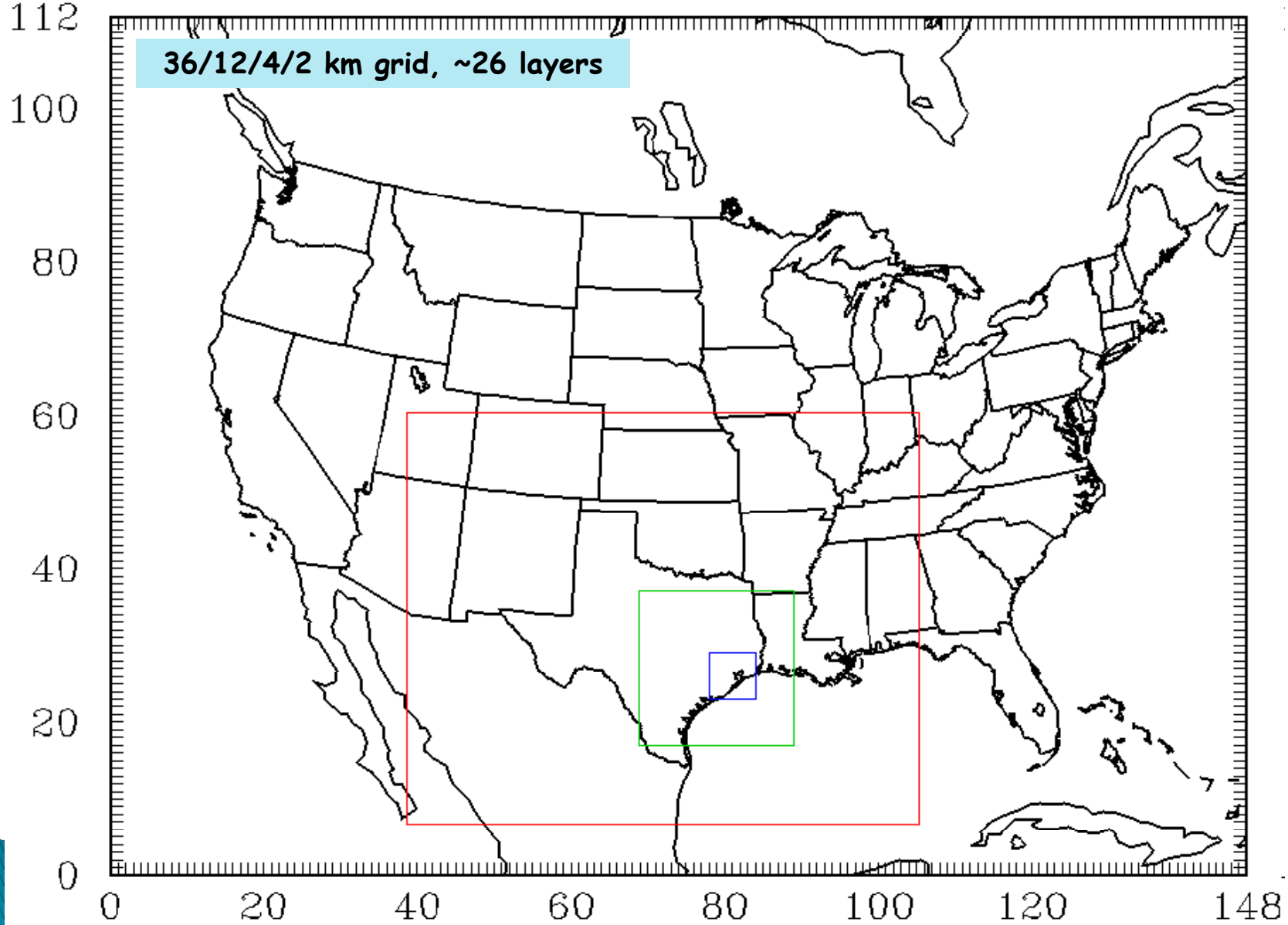
8hrC Modeling Domain



Multi-Scale Ensemble Tools

- Emissions:
  - SMOKE using MEGAN
  - SMOKE using BEIS (or GloBEIS)
  - SMOKE using alternate MV methodology including MOVES
- Meteorology:
  - WRF (2-3 alternate science configurations)
- Photochemical-Aerosol:
  - CAMx
  - CMAQ
- Condensed Chemical Mechanism:
  - CB06
  - SAPRC07

Base Years Modeling Approach

- Construct extended ozone season (7 months) base cases for 2009, 2010, & 2011 at nested 36/12/4/2 grid domains.
- Using ambient measurements, separate base case days at each monitor into two (or more) categories of ozone formation/control characteristics:
  - **Category I Days**: Periods for which ozone dynamics <u>are adequately represented</u> in contemporary emissions inventorying and transport science methods.
  - **Category II Days**: Periods reflecting emissions phenomena, chemical processing, or transport patterns <u>cannot be represented</u> by present model science formulations and/or input data sets.
- Apply multi-scale ensemble modeling techniques to Category I days, evaluate model performance, and calculate bias minimization statistics for future year ozone simulations.
- For Category II days, develop and apply tailored WoE modeling techniques such as case studies of plausible event emissions, Process Analysis, and DDM and lateral boundary condition sensitivity simulations.

Future Years Modeling Approach

- Construct future year ozone season (7 months) base cases for 3-yr period prior to HBG attainment date (2018, 2020, 2025?).
- Apply best performing ensemble models to future Category I days.
- Apply tailored WoE modeling techniques to future Category II days.
- At each monitor calculate O3 NAAQS attainment metrics (3-year avg. of the 4th highest daily max. 8-hour ozone & the seasonal W126 ozone concentration.
- Determine whether 4th highest value at a monitor is most effectively reduced by
  - Applying emissions controls to Cat I days
  - Performing case-by-case, weight of evidence modeling of controls on Cat II days
  - Testing control strategy reductions in both ‘typical’ and ‘case by case’ modes.

Attainment Estimation

- Default Guidance – Use the 2009-2011 base and future projection episodes to calculate RRFs and apply the EPA attainment equation (DV_f=RRF*DV_b) to compare with the 8hrC WOE procedure, below…

8hrC WOE Attainment Estimation Approach…

- 1. Direct Numerical Simulation of Cat I Days – Multi-scale ensemble simulation of three sequential 7-month long summer ozone seasons in Texas immediately preceding attainment year. (DV_f calculated as 3-yr average of 4th highest MDA8 at each monitor *for Cat I days only*).

- 2. WoE Simulations for Cat II Days – Model potential emissions control effectiveness at monitors whose 4th highest ozone level, in one or more future years, falls *within the Cat II classification.*

- 3. Construct WoE Attainment Estimate – Calculate 3-yr avg. of 4th highest projected O_3 at each monitor, merging results from steps 1 and 2.

Recent Research Findings

- Ozone Process Dynamics (formation & control)
- Multi-Scale Ensemble Modeling Methods
  - Science Improvements
  - Ensemble Model Evaluation
  - Bias Adjustments (base & future)
  - Deterministic & Probabilistic Interpretations
- Ozone NAAQS Attainment Estimation
  - Historical Approach
  - New Methods

Ozone Process Dynamics

- Vizuete, W. et al., (2010). “Evaluation of relative response factor methodology for demonstrating attainment of ozone in Houston, TX”, *J. of Air & Waste Management Assoc*., **60**, pp 838-848.

- Vizuete, W. et al., (2010). “8-hr ozone attainment demonstration: Conceptual approaches and recent experiences in Houston, TX”, *J. of Air & Waste Management Assoc*., (in press).

- Henderson, B. et al., (2010). “The influence of model resolution on ozone in industrial volatile organic compound plumes”, *J. of Air & Waste Management Assoc*., (in press).

Multi-Scale Ensemble Modeling

- Multi-Model Ensembles (MME) -- Simulations produced by alternative configurations of emissions, meteorological, chemical, and geophysical modules. (Wilczak et al., 2009; Djalalova et al., 2010).

- Single-Model Ensembles (SME) -- Simulations produced by a single air quality model supplied with a range of inputs covering emissions estimates, chemical reaction schemes, meteorological data, etc. (Pinder et al., 2009; Galmarini et al., 2010; Tian et al., 2010).

Key Implementation Questions

- **Model Testing**: What are optimal base year evaluation methods, metrics, & displays?

- **Bias Adjustment**: Is a quantile-based approach the best choice for ameliorating bias in base case and future year ensemble member predictions? Implemented on a monitor- and day- specific basis?

- **Multi-Model Combination**:
  - What specific metrics inform whether a model is 'fit' for use in future projections?
  - Should ensemble members be weighted based on performance? (Weigel et al., 2010)
  - Should poor performing ensemble members be dropped?

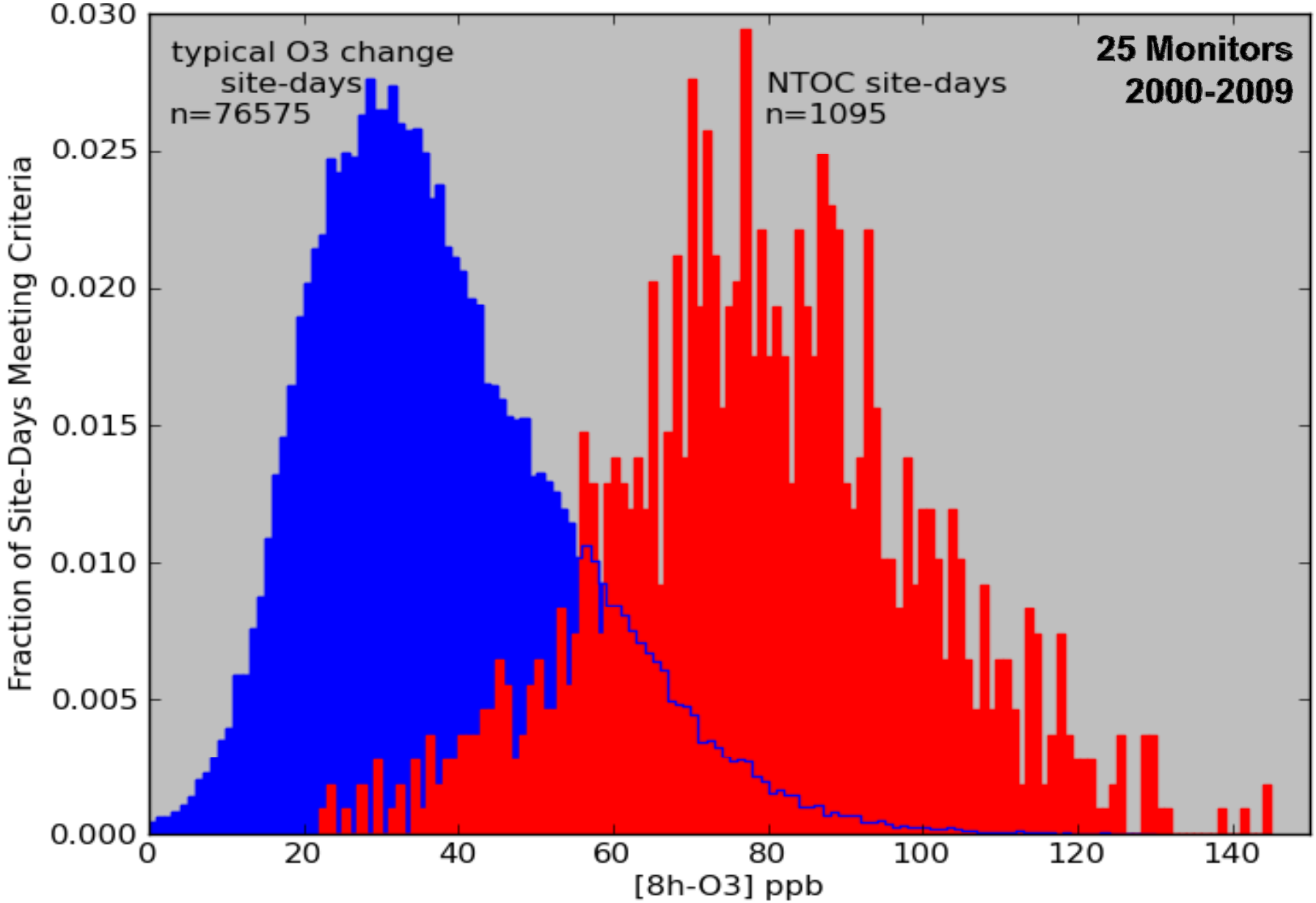
- **Combining Category I and II Days**: How should ensemble results for Cat I days be combined with case-by-case, WOE calculations for Cat II days at 'problem' monitors?

- **Model Output:** What are the most relevant policy & science metrics to distill from future year simulations? (Monitor-specific vs. estimates at every point in space (median, mean, maximum, time integrated…)

References

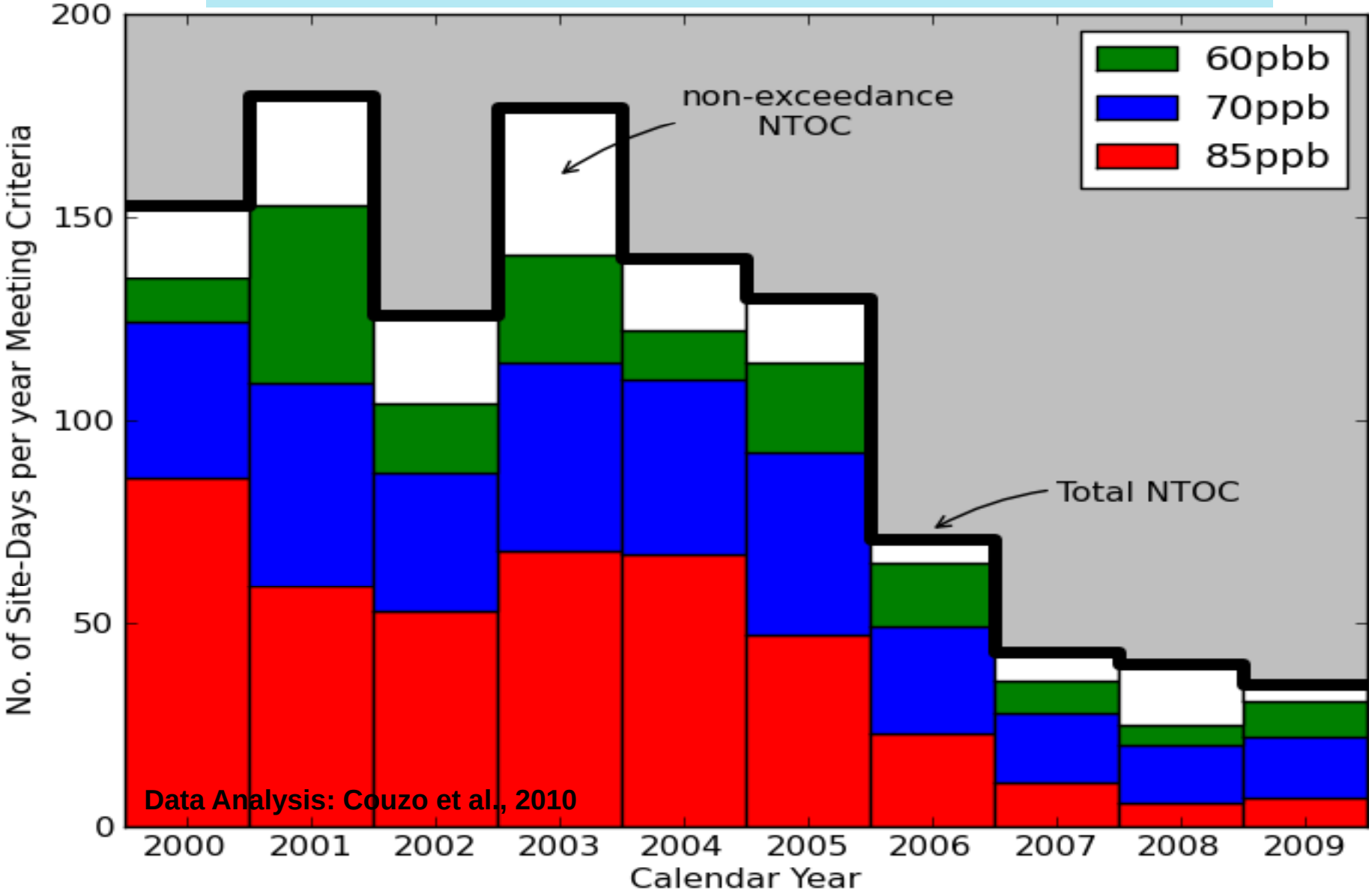
- Djalalova, I. et al., 2010. Ensemble and bias-correction techniques for air quality model forecasts of surface O_3 and $PM_{2.5}$ during the TexAQS-II experiment of 2006. *Atmos. Environ.* **44,** 455-467.
- Galmarini, S., et al., 2010. Multi-model vs. EPS-based ensemble atmospheric dispersion simulations: A quantitative assessment on the ETEX—1 tracer experiment case. *Atmos. Environ.* **44,** 3558-3567.
- Kang, D. et al., 2010. Real-time bias-adjusted O_3 and $PM_{2.5}$ air quality index forecasts and their performance evaluations over the continental United States. *Atmos. Environ.* **44,** 2203-2212.
- Li, H. et al., 2010. Bias correction of monthly precipitation and temperature fields from IPC AR4 models using equidistant quantile matching, *J. Geophys. Res*., **115**, D10101.
- Pinder, R. W., et al., 2009. Efficient probabilistic estimates of surface ozone concentration using an ensemble of model configurations and direct sensitivity calculations, *Environ. Sci. Tech.,* **43**, 2388-2393.
- Tian, D., et al., 2010. Uncertainty analysis of ozone formation and response to emissions controls using higher-order sensitivities, *J. Air & Waste Manage. Assoc.,* **60**, 797-804.
- Weigel, A., et al., 2010. Risks of model weighting in multi-model climate projections, *J. Climate,* (in press).
- Wilczak, J. M., et al., 2009. Analysis of regional meteorology and surface ozone during the TexAQS II field program and an evaluation of the NMM-CMAQ and WRF-Chem air quality models, *J.. Geophys. Res.,* **114**.

Distribution of Cat I (Typical) & Cat II (NTOC) Days in HGB



CAT II O_3 Exceedances Are Declining Significantly

Tailored strategies for reducing 4th highest Cat II day impacts may avoid unnecessary or ineffective controls arising from default EPA methodology.



Data Analysis: Couzo et al., 2010