Development of an Ozone Screening Tool for the Midwest

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Motivation

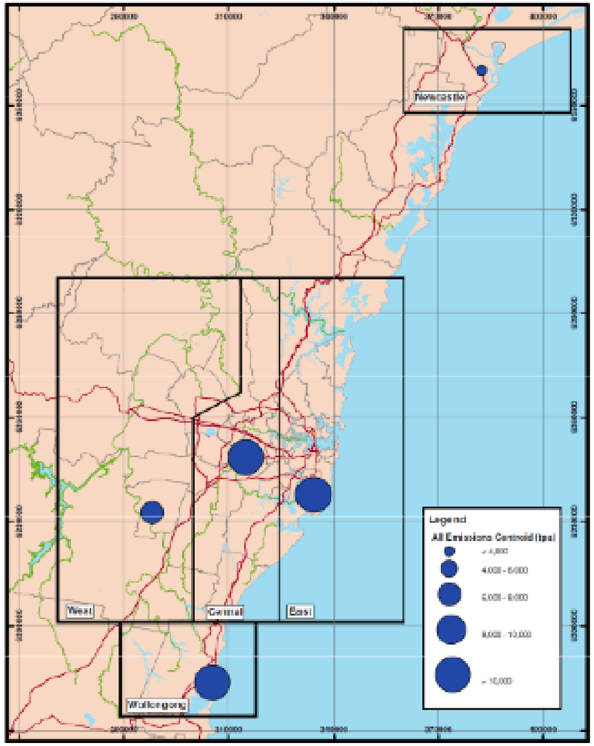
- July 2010 - Sierra Club petitions EPA to designate air quality models for PSD permitting
- January 2012 – EPA grants Sierra Club's petition and commits to updating the *Guideline on Air Quality Models* (Appendix W)
- Regional photochemical modeling is best science for addressing ozone impacts, but computational intensive and impractical for routine permitting
- Regulators would like an easy to use screening tool to assess the ozone impact of stationary sources for PSD permitting applications

Reduced Form Models

- Use regional photochemical model results to develop a simplified localized framework
  - Equivalency Ratio (Margaret McCourtney, MPCA)
  - Interpollutant Trading Ratios (James Boylan, Georgia EPD)
  - Response Surface Model (Carey Jang, EPA)
  - Parametric Model (Greg Yarwood, ENVIRON)

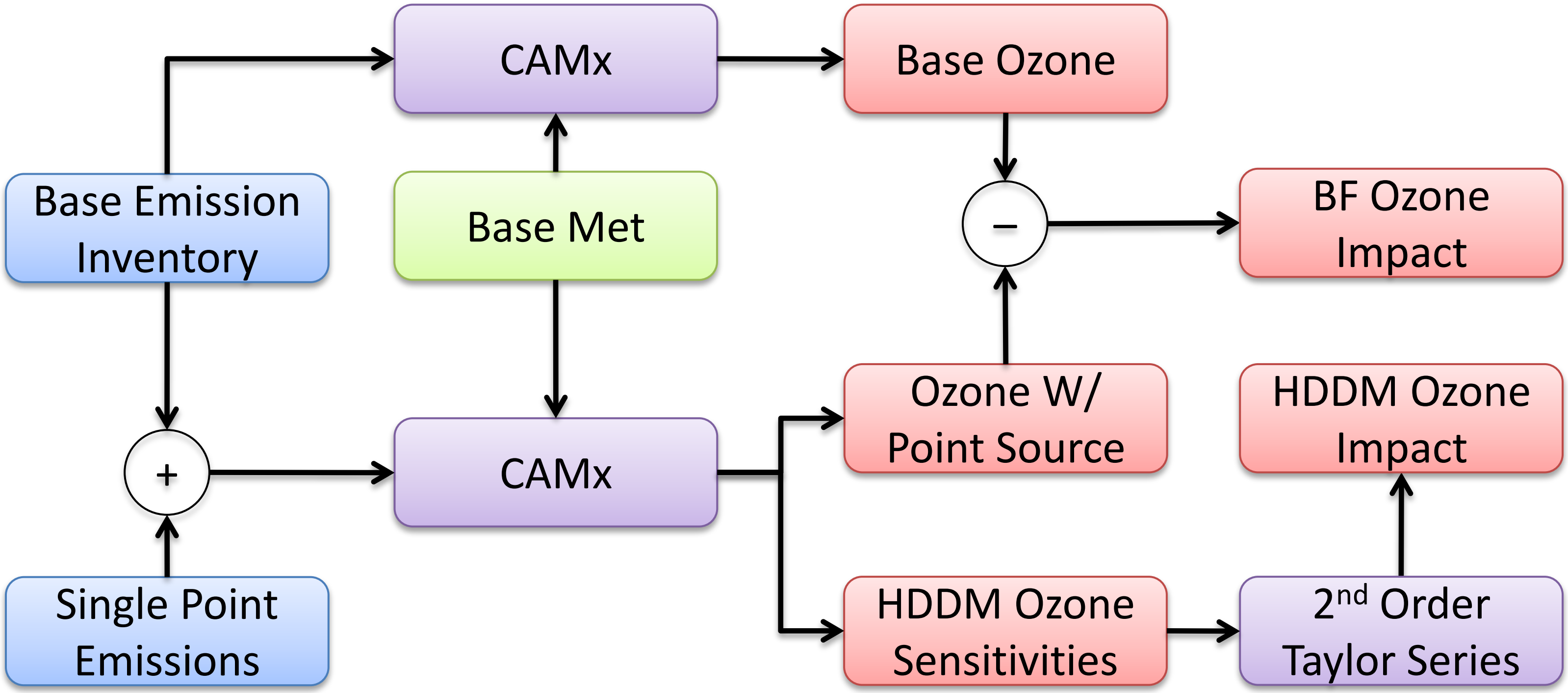
Background

- Parametric Model (Yarwood, 2011)
  - – Screening tool developed for Sydney
    - 3 Km CAMx higher-order direct decoupled method (HDDM) simulations of the summer
    - Assumptions:
      - – Ground source
      - – Located at center of emissions by mass



Yarwood, G., Scorgie, Y., Agapides, N., Tai, E., Karamchandani, P., Bawden, K., Spencer, J., Trieu, T, 2011. **A screening method for ozone impacts of new sources based on high-order sensitivity analysis of CAMx simulations for Sydney**. Proceedings, *10th Annual CMAS Conference, Chapel Hill, NC.*

Background



Base Emission Inventory

Single Point Emissions

+

CAMx

Base Met

CAMx

Base Ozone

−

Ozone W/ Point Source

HDDM Ozone Sensitivities

BF Ozone Impact

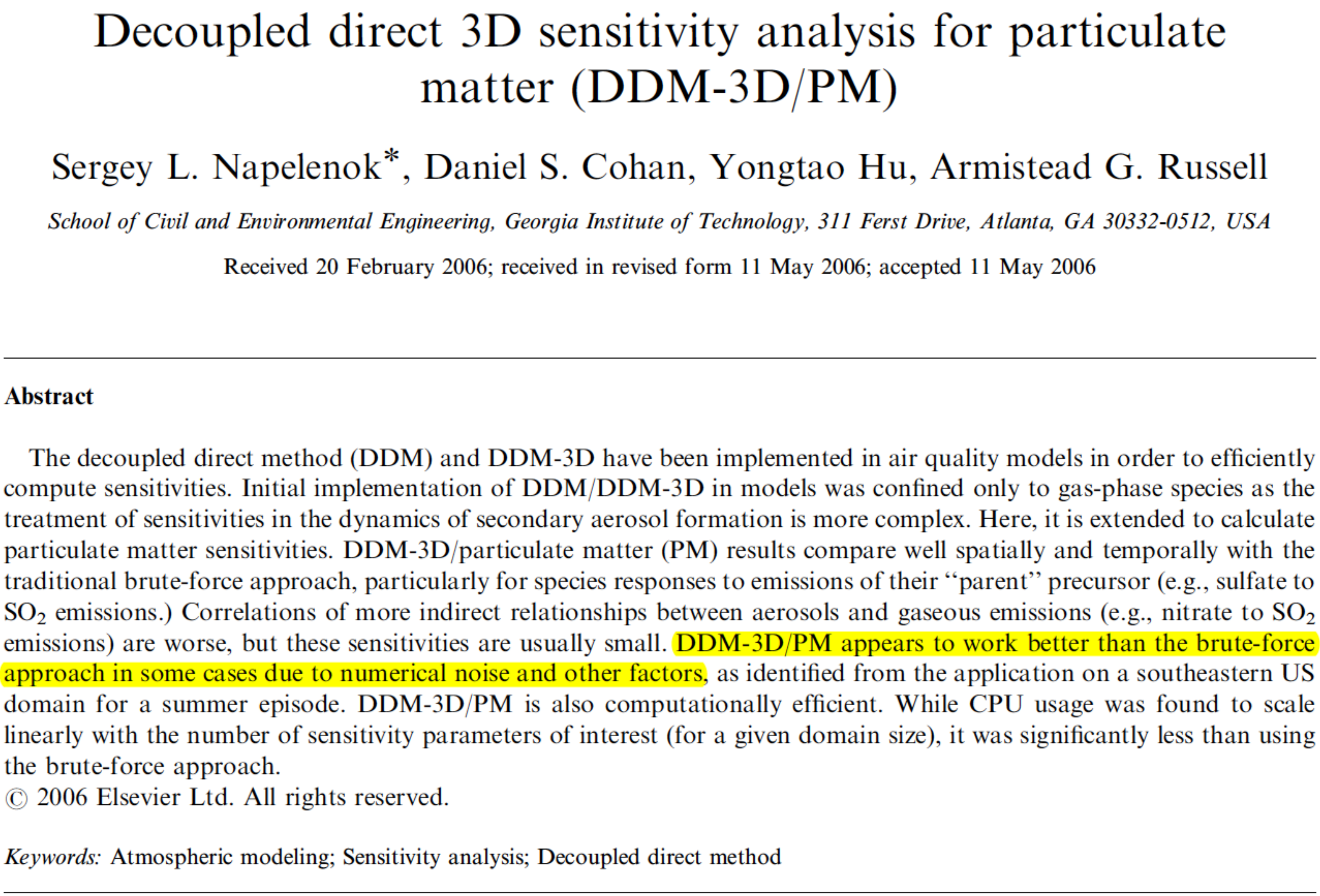
HDDM Ozone Impact

2nd Order Taylor Series

2nd order Taylor series

$$\nabla[O_3] = \nabla E_{NO_X}\frac{\partial[O_3]}{\partial E_{NO_X}} + \nabla E_{VOC}\frac{\partial[O_3]}{\partial E_{VOC}} + \frac{1}{2}\left(\nabla E_{NO_X}^2 \frac{\partial^2[O_3]}{\partial E_{NO_X}^2} + \nabla E_{VOC}\nabla E_{NO_X}\frac{\partial^2[O_3]}{\partial E_{VOC}\partial E_{NO_X}} + \nabla E_{VOC}^2\frac{\partial^2[O_3]}{\partial E_{VOC}^2}\right)$$

Background



Decoupled direct 3D sensitivity analysis for particulate matter (DDM-3D/PM)

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Abstract

The decoupled direct method (DDM) and DDM-3D have been implemented in air quality models in order to efficiently compute sensitivities. Initial implementation of DDM/DDM-3D in models was confined only to gas-phase species as the treatment of sensitivities in the dynamics of secondary aerosol formation is more complex. Here, it is extended to calculate particulate matter sensitivities. DDM-3D/particulate matter (PM) results compare well spatially and temporally with the traditional brute-force approach, particularly for species responses to emissions of their "parent" precursor (e.g., sulfate to SO_2 emissions.) Correlations of more indirect relationships between aerosols and gaseous emissions (e.g., nitrate to SO_2 emissions) are worse, but these sensitivities are usually small. DDM-3D/PM appears to work better than the brute-force approach in some cases due to numerical noise and other factors, as identified from the application on a southeastern US domain for a summer episode. DDM-3D/PM is also computationally efficient. While CPU usage was found to scale linearly with the number of sensitivity parameters of interest (for a given domain size), it was significantly less than using the brute-force approach.

Keywords: Atmospheric modeling; Sensitivity analysis; Decoupled direct method

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Problem Statement

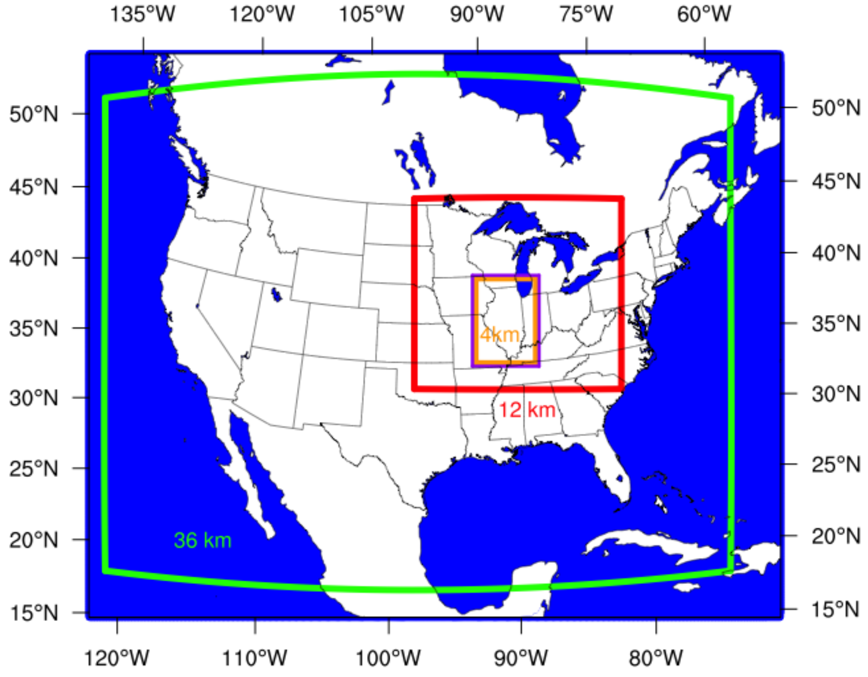
- **Question**: How do ozone sensitivities to emission rates vary with emission rate and stack characteristics?

- **Approach**: Use multiple CAMx HDDM simulations of individual point sources to train a statistical model to empirically relate

$$S = f\left(E_{NO_X}, E_{VOC}, SH, \nabla x, \nabla y\right)$$

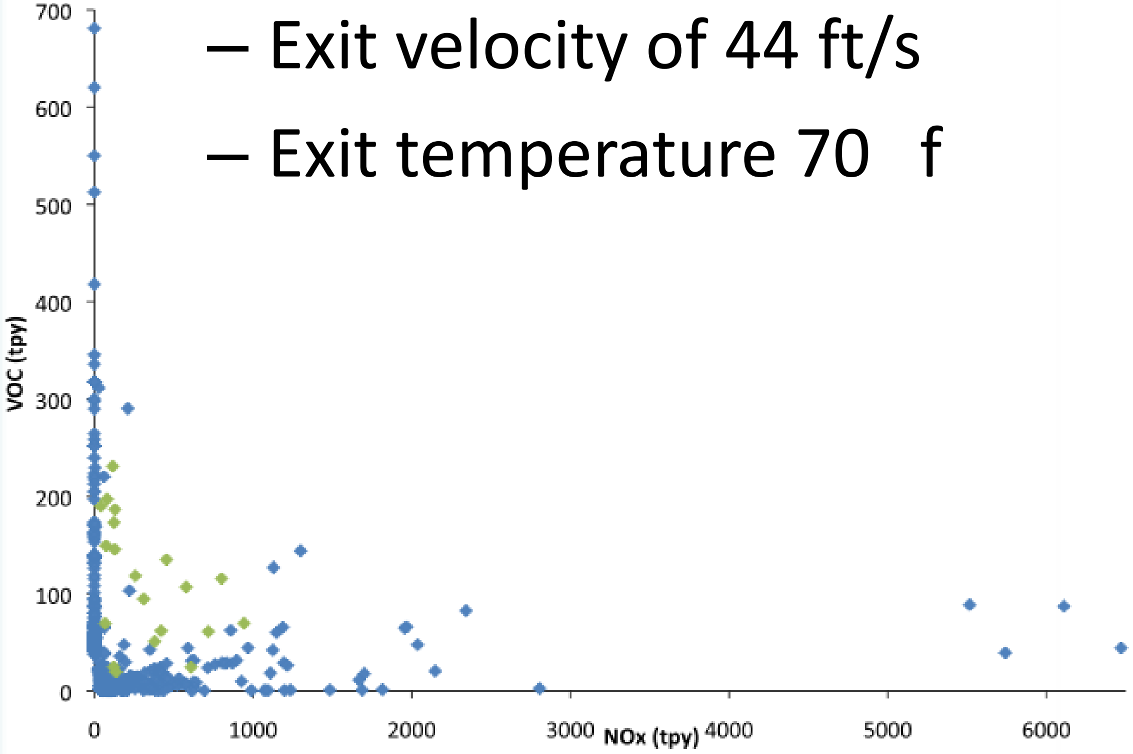
Methodology

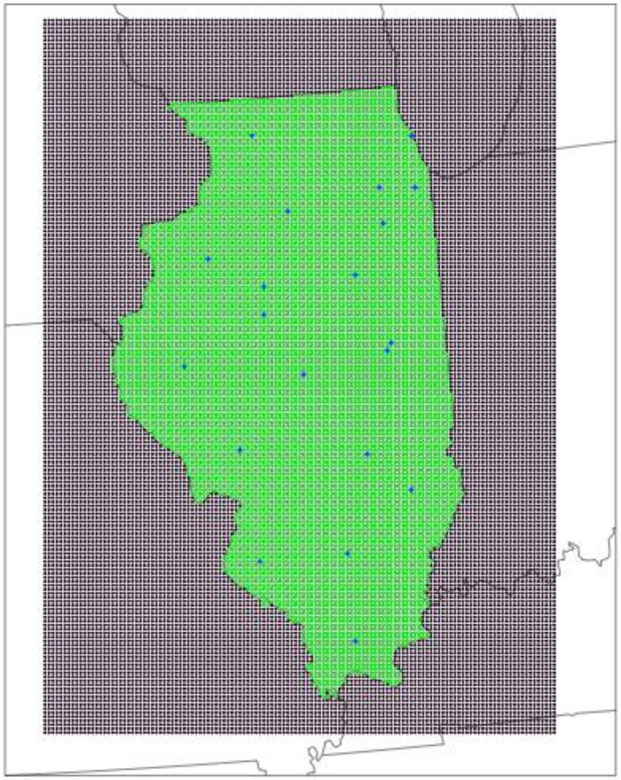
- Proof of concept conducted for test case in Illinois
- Based on LADCO 2007 Modeling platform
- 4 km CAMx HDDM modeling of summer 2007



Methodology

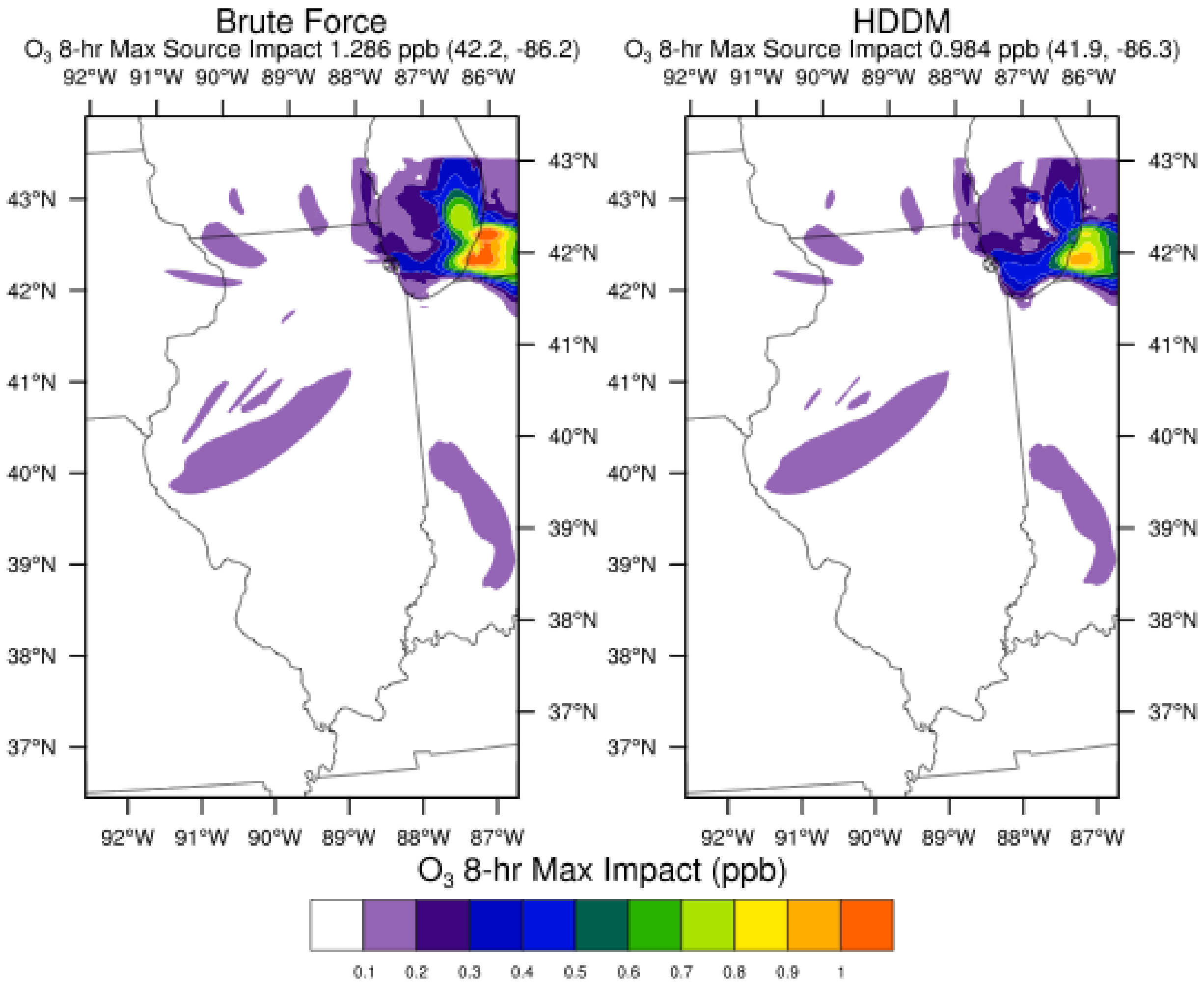
- 20 hypothetical point sources modeled with HDDM
  - Stack diameter is linearly related to stack height (SH)
  - Exit velocity of 44 ft/s
  - Exit temperature 70 f





Training Data Point 2

E_{NOx} = 718 tpy, E_{VOC} = 61 tpy, SH = 120 ft



Brute Force

O_3 8-hr Max Source Impact 1.286 ppb (42.2, -86.2)

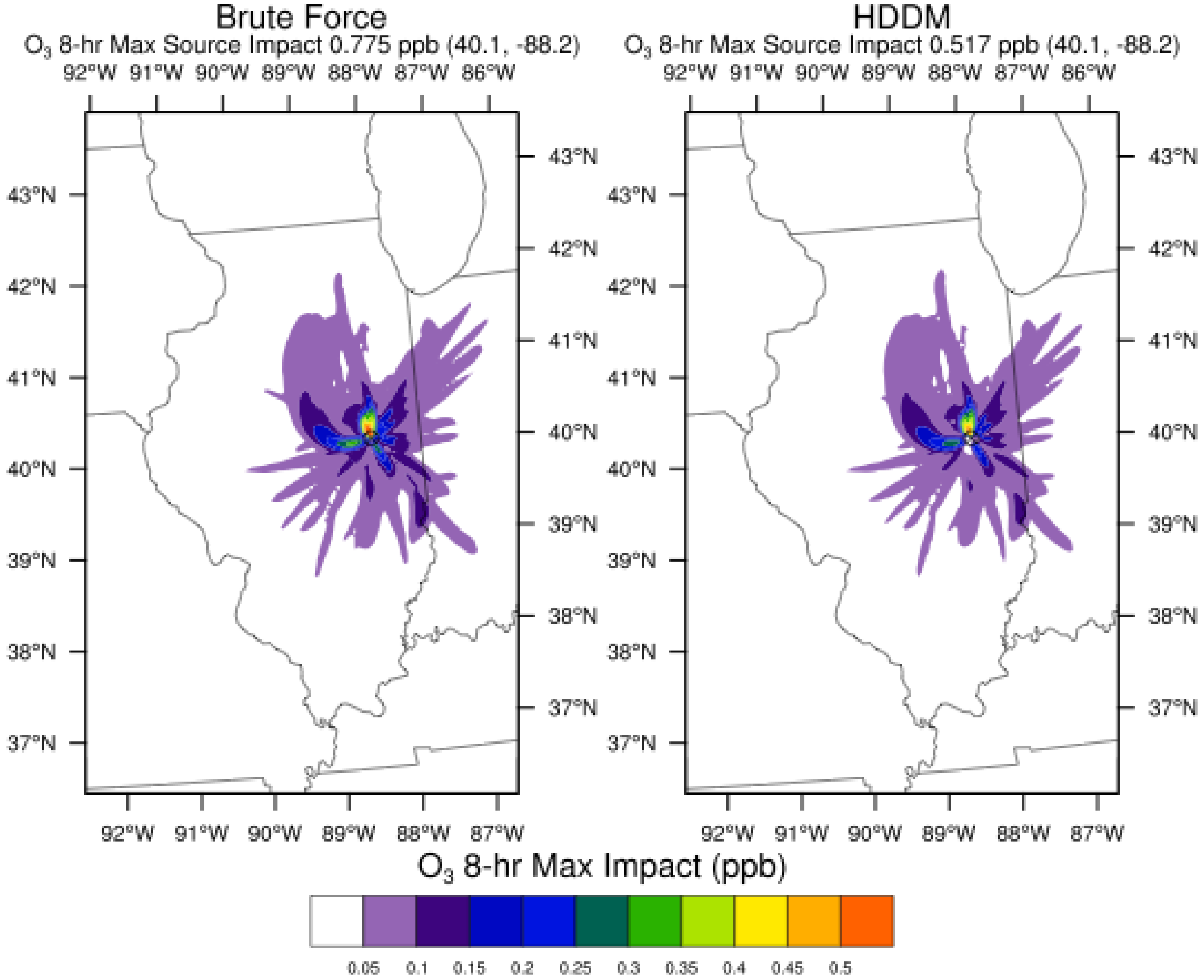
HDDM

O_3 8-hr Max Source Impact 0.984 ppb (41.9, -86.3)

O_3 8-hr Max Impact (ppb)

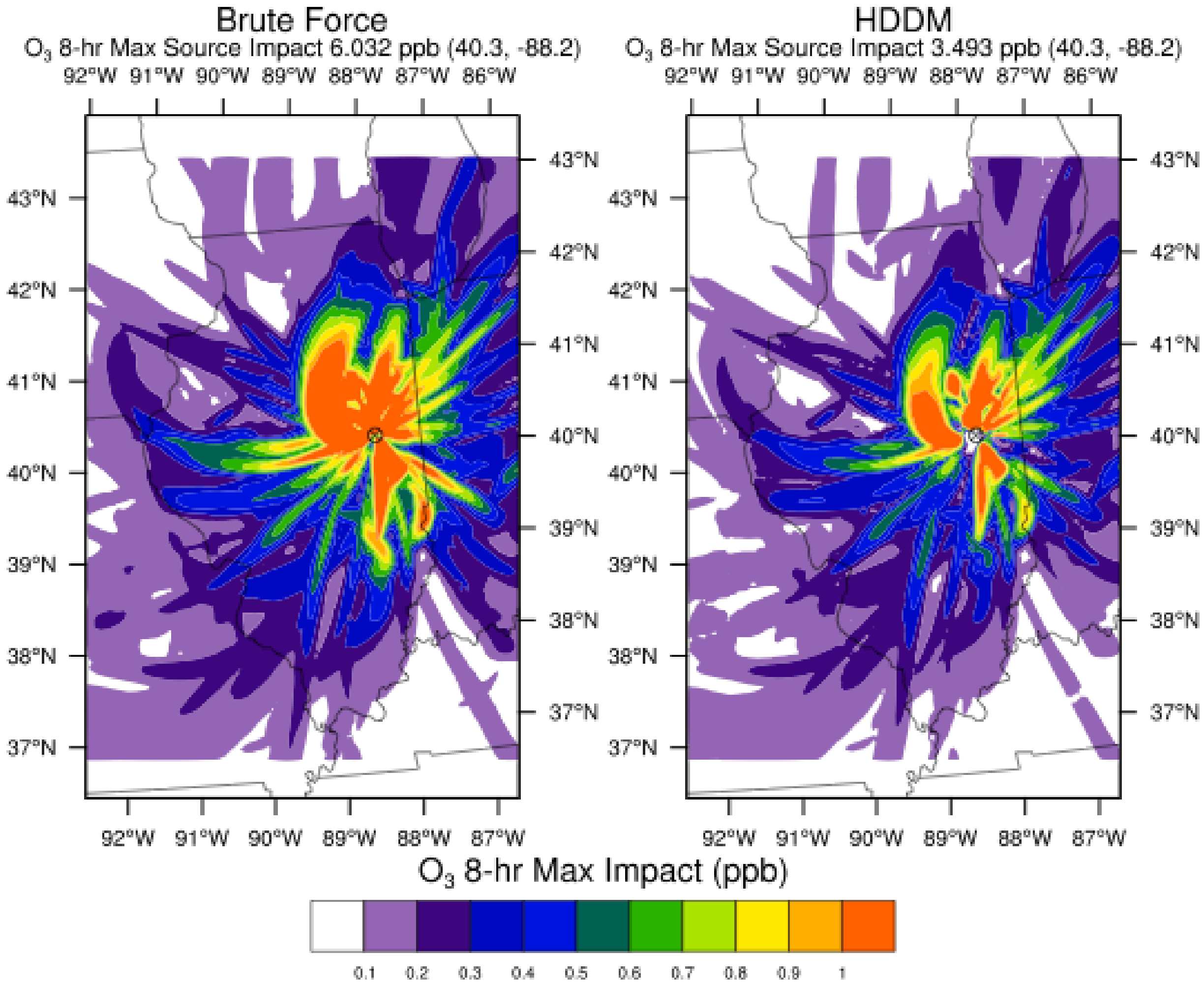
Training Data Point 5

E_{NOx} = 80 tpy, E_{VOC} = 197 tpy, SH = 48 ft



Training Data Point 6

E_{NOx} = 943 tpy, E_{VOC} = 70 tpy, SH = 454 ft



Brute Force

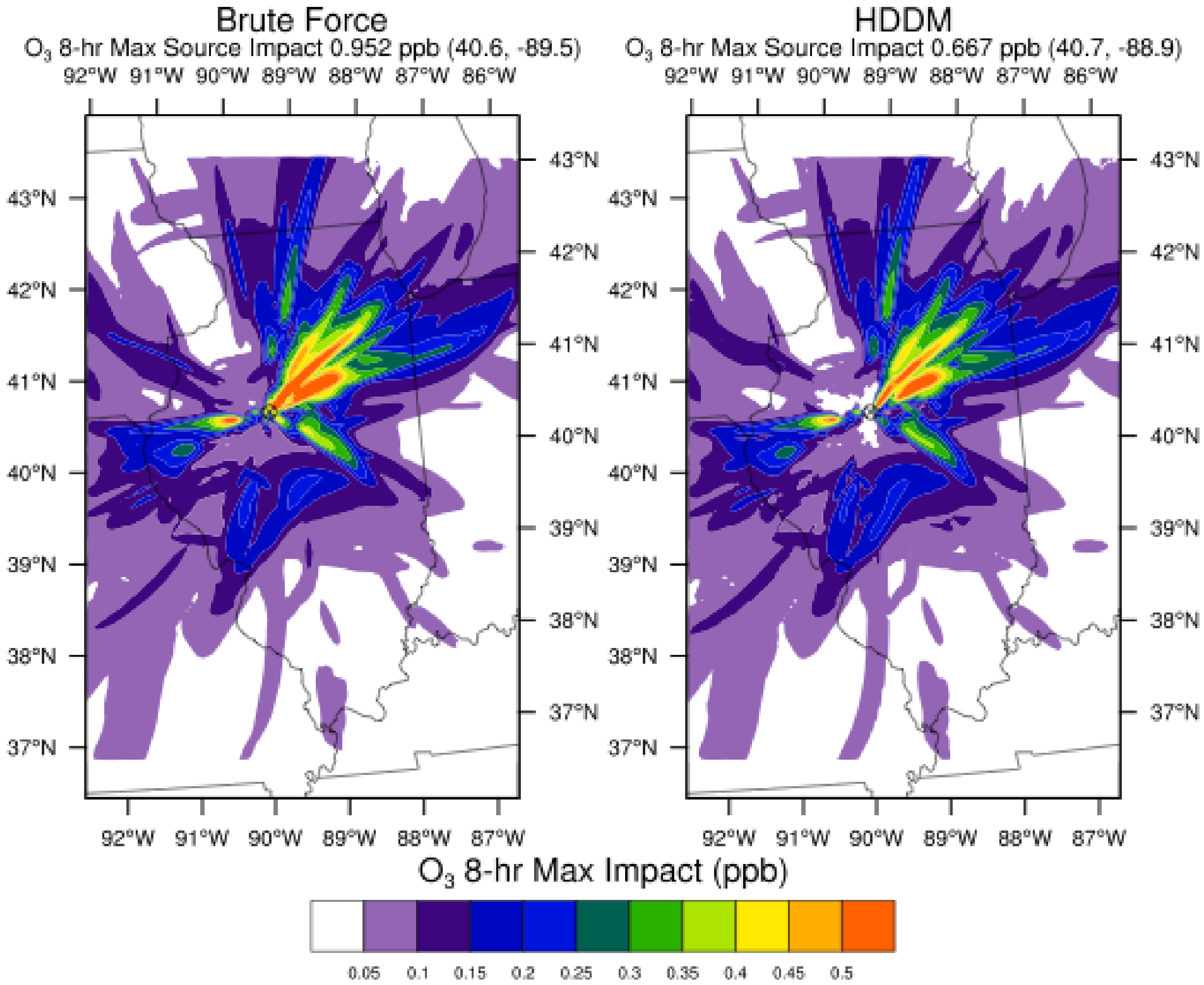
O_3 8-hr Max Source Impact 6.032 ppb (40.3, -88.2)

HDDM

O_3 8-hr Max Source Impact 3.493 ppb (40.3, -88.2)

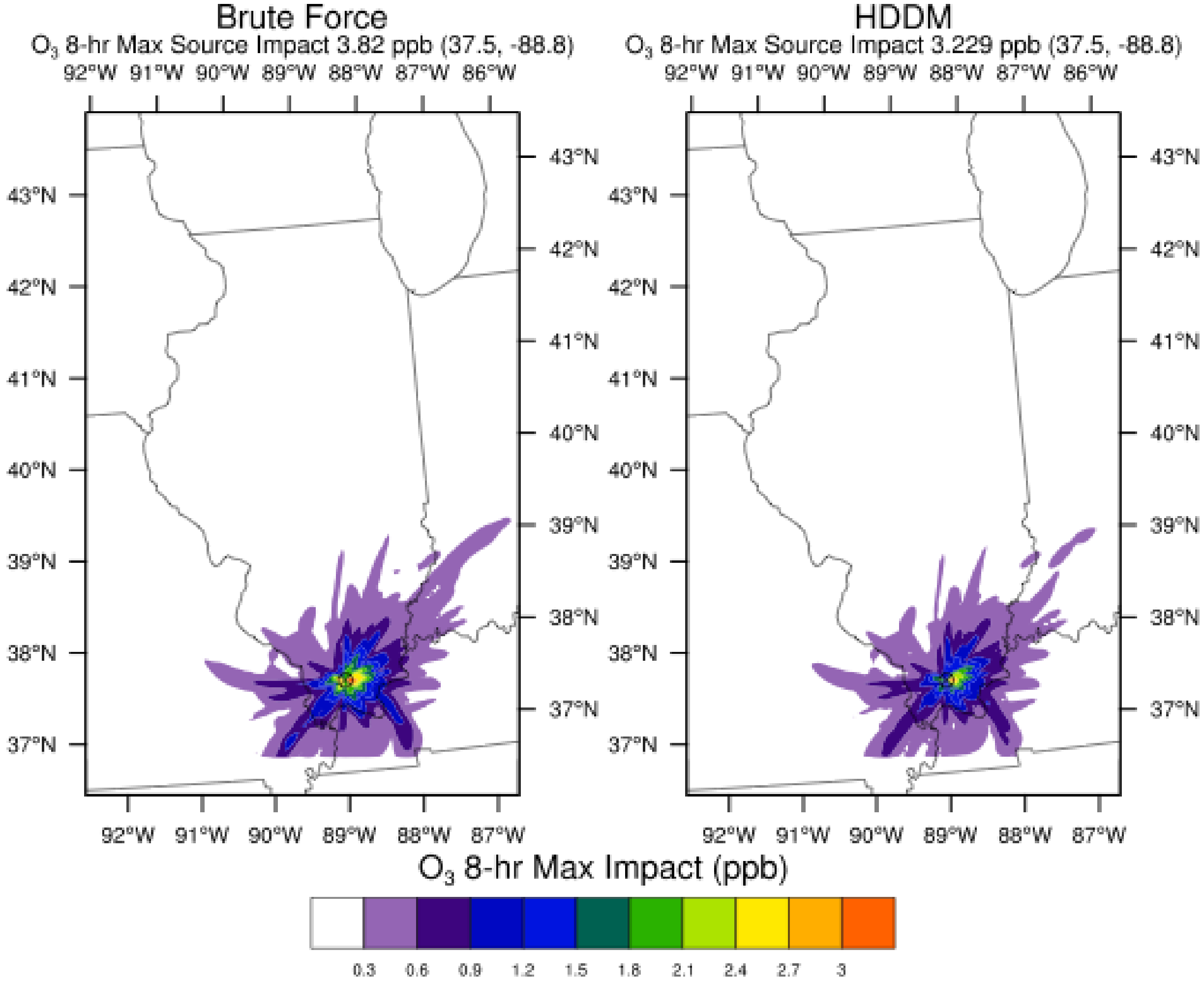
Training Data Point 9

E_{NOx} = 610 tpy, E_{VOC} = 25 tpy, SH = 194 ft



Training Data Point 18

E_{NOx} = 380 tpy, E_{VOC} = 51 tpy, SH = 268 ft

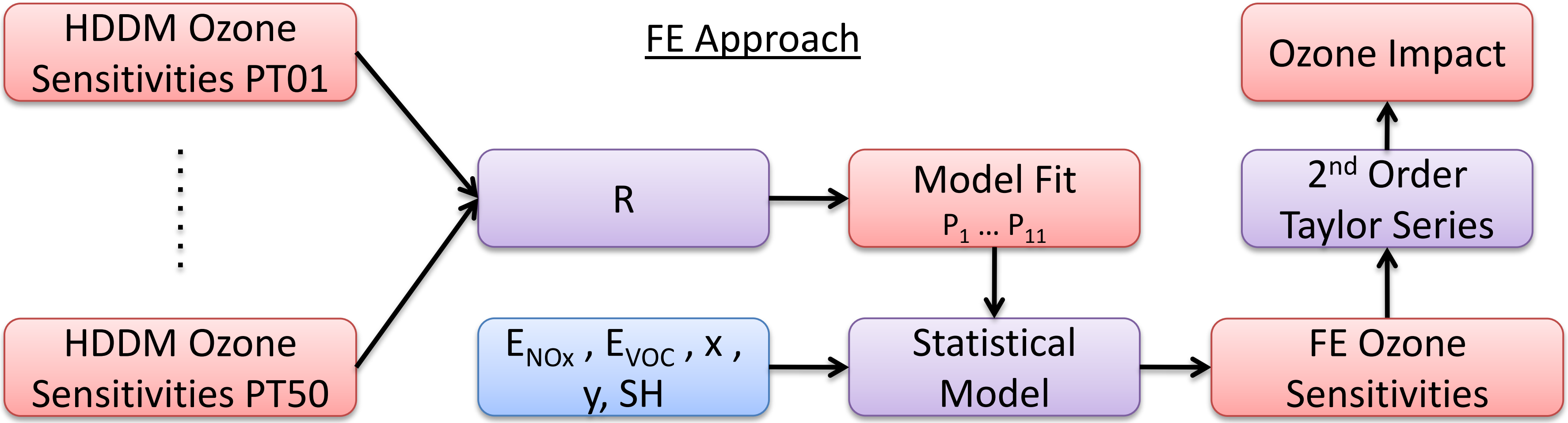


Summary

- FE matches HDDM training data well
- FE/HDDM matches BF in magnitude and extent of impact, however BF produces a higher peak impact
- FE Model would benefit from additional training data

Methodology

FE Approach



HDDM Ozone Sensitivities PT01

⋮

HDDM Ozone Sensitivities PT50

R

Model Fit $P_1 \ldots P_{11}$

E_{NOx} , E_{VOC} , x , y, SH

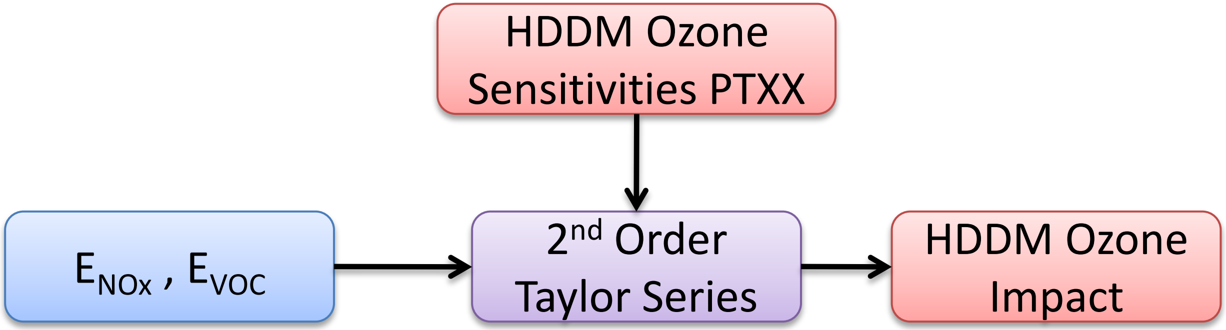
Statistical Model

FE Ozone Sensitivities

2nd Order Taylor Series

Ozone Impact

HDDM Approach



HDDM Ozone Sensitivities PTXX

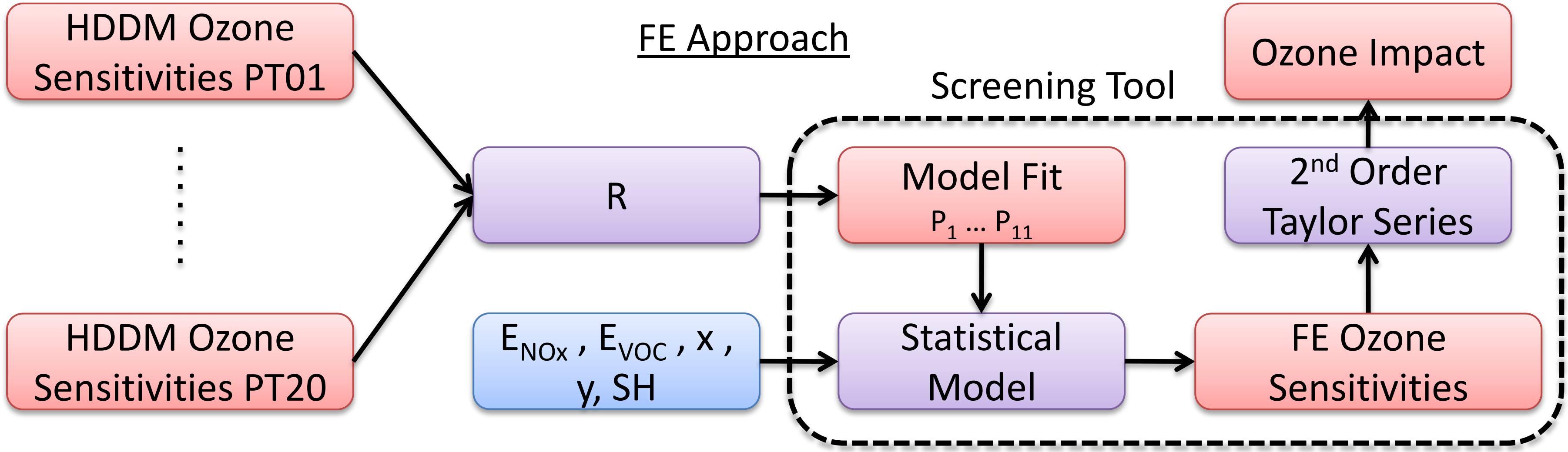
E_{NOx} , E_{VOC}

2nd Order Taylor Series

HDDM Ozone Impact

Methodology

FE Approach



HDDM Ozone Sensitivities PT01

⋮

HDDM Ozone Sensitivities PT20

R

E_{NOx} , E_{VOC} , x , y, SH

Screening Tool

Model Fit

$P_1 \dots P_{11}$

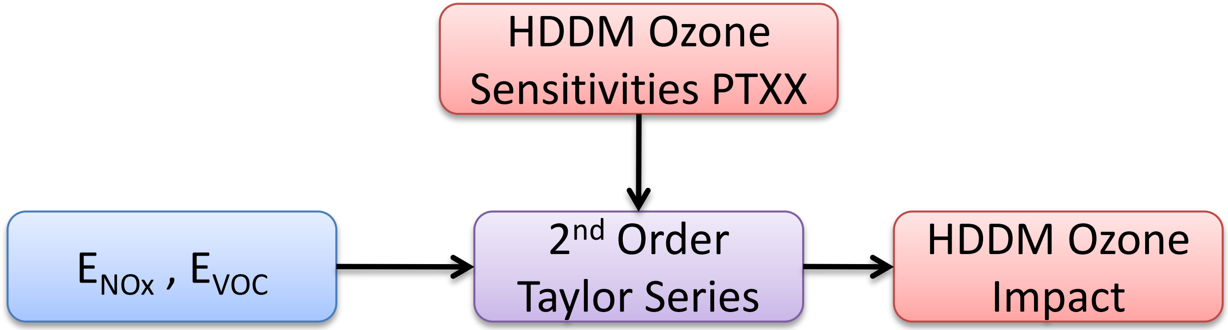
Statistical Model

FE Ozone Sensitivities

2nd Order Taylor Series

Ozone Impact

HDDM Approach



HDDM Ozone Sensitivities PTXX

E_{NOx} , E_{VOC}

2nd Order Taylor Series

HDDM Ozone Impact

Statistical Models

- Potential statistical models
  - CART
  - Neural network
  - Kriging
  - Fixed-Effects
  - Response Surface Model

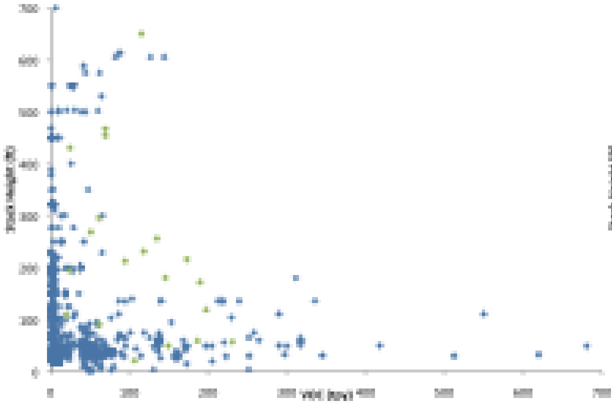
Future Work

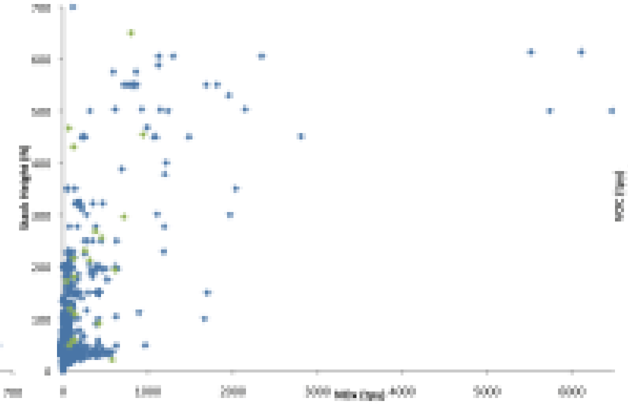
- Investigate differences in peak impact predicted from BF and HDDM
- Implement multivariate universal cokringing
  - Accounts for covariance among HDDM sensitivities
- Examine different VOC profiles
- Explore other statistical models
- Apply methodology to develop PM screening tool

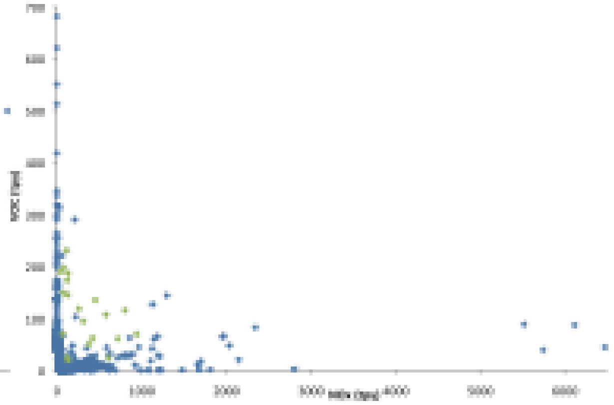
Acknowledgments

- Scott Leopold – IL EPA
- Greg Yarwood – ENVIRON
- Kirk Baker – OAQPS
- Margaret McCourtney – MN PCA
- Randall Robinson – EPA Region 5
- Mark Derf – IN DEM

20 HDDM Modeled Point Sources

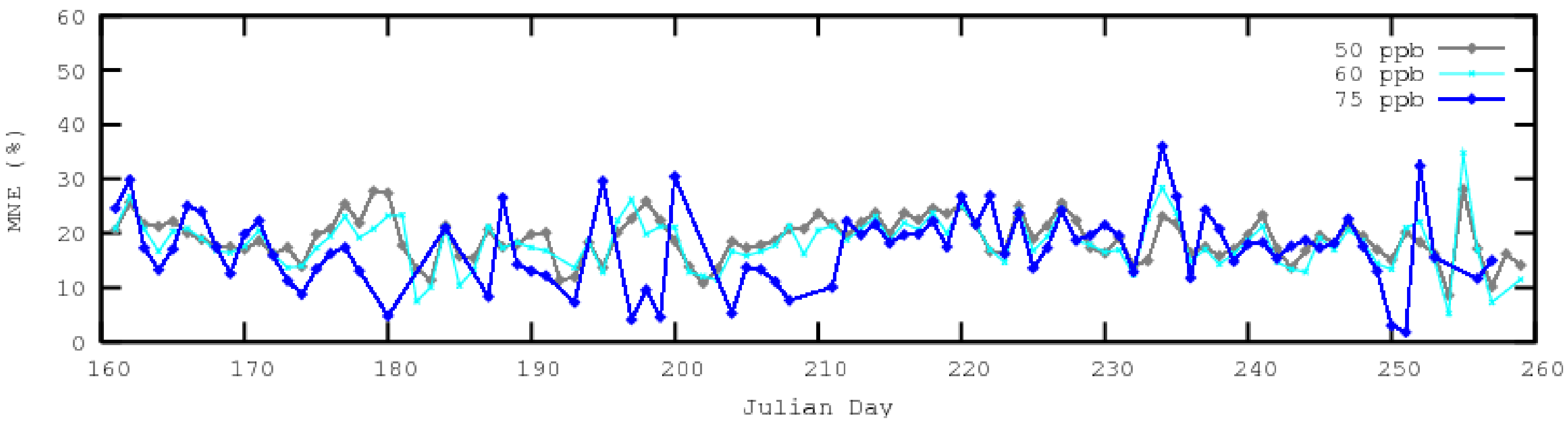




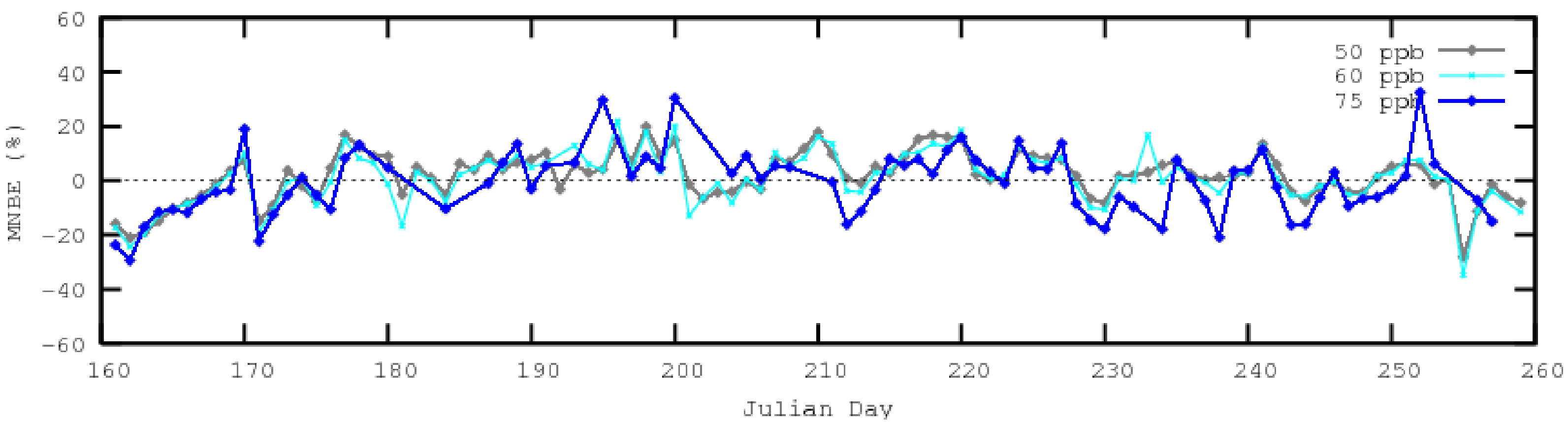


LADCO 2007 Modeling Platform

- Ozone Performance



8 HR O3 (ppb) - 2007 - baseDv3_M1_07summer [LADCO] camx



8 HR O3 (ppb) - 2007 - baseDv3_M1_07summer [LADCO] camx