

Application of Direct Decoupled Method (DDM) for the TCOPS field study period

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**Presentation for NWAIRQUEST Meeting
June 15, 2016**

How does the model respond to a change in an independent parameter?

- **“Brute-Force” Method:**

- Run model once for a “base case”
- Change the initial input and run model again for each of N perturbations (the response of ozone to a change in the initial amount of an individual VOC is estimated)
- Involves one at-a-time parameter perturbation
- Quickly becomes inefficient as a large number of sensitivity coefficients need to be computed
- A small perturbation may result in a signal that is hard to separate from numerical noise.

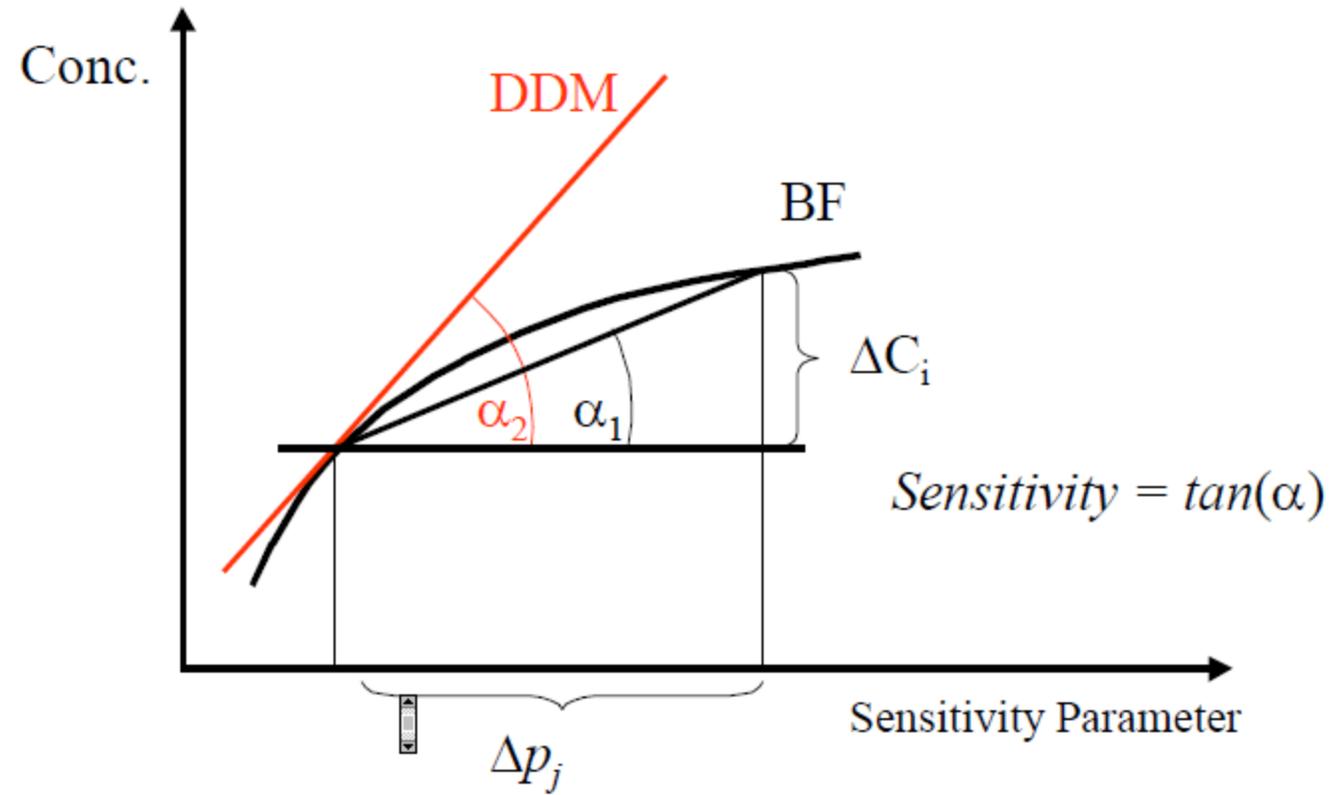
$$S_n = \frac{C_n - C_0}{P_n - P_0}$$

Sensitivity Methods

- Direct Coupled Method: (Dickerson et al., 1982)
- Green's function: (Rabitz et al., 1983)
- **Direct Decoupled Method:** (Dunker 1981, Yang et al., 1997)
 - ❖ Sensitivity equations are derived directly from model equations and are solved decoupled from concentrations.
 - ❖ DDM-3D calculates sensitivities simultaneously with concentrations calculations
 - ❖ The local sensitivity of a model output to a parameter is equal to the partial derivative of the output with respect to the parameter

$$S_n = \frac{\partial C}{\partial p_n}$$

DDM vs. Brute-Force



atmospheric diffusion equation (ADE)

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot (\mathbf{u}C_i) + \nabla \cdot (\mathbf{K}\nabla C_i) + R_i + E_i,$$

Perturbation

$$p_j = \epsilon_j P_j = (1 + \Delta\epsilon_j) P_j$$

semi-normalized first-order sensitivity coefficients

$$\mathbf{S}_j^{(1)} = P_j \frac{\partial \mathbf{C}}{\partial p_j} = P_j \frac{\partial \mathbf{C}}{\partial (\epsilon_j P_j)} = \frac{\partial \mathbf{C}}{\partial \epsilon_j}$$

The sensitivity equation

$$\frac{\partial S_{ij}}{\partial t} = -\nabla \cdot (\mathbf{u}S_{ij}) + \nabla \cdot (\mathbf{K}\nabla S_{ij}) + \mathbf{J}S_{ij} + E_j \delta_{ij},$$

u: the three-dimensional wind field

K: the turbulent diffusivity tensor.

C: grid average concentration

E: emission rate

R: chemical reaction rate of species i

S_{ij}: the semi-normalized sensitivity of species i to the emissions of species j

J: the Jacobian matrix of the reaction rates

δ_{ij}: the Kronecker delta function.

ε: scaling variable

Extending Sensitivities Results

- ❖ Many studies have assumed that responsiveness of concentrations to one amount of emissions perturbation could be linearly extrapolated to estimate response to other amounts of perturbation.
- ❖ First order sensitivity : perturbation up to 30% (Dunker et al. (2002))
- ❖ Second order sensitivity: perturbation up to 50% (Napelenok et al. (2011))

CMAQ-DDM-3D (v5.0.2)

DDM-3D uses the same numerical algorithms for transport-related processes (advection, diffusion, deposition, etc.) as for concentrations.

Processes that are not linear, such as aerosol formation and cloud dynamics, are treated slightly differently.

- ✓ CMAQ-DDM-3D generates concentration outputs that are essentially *identical* to normal CMAQ results, while simultaneously computing sensitivity coefficients for any species concentration to a change in
 - initial conditions,
 - boundary conditions,
 - emission rates.
- ✓ CMAQ-DDM-3D requires the same input files as a normal CMAQ run. Additional input files may be required depending on the choice of calculated sensitivity parameters.

File	Type	Contains	Base model analog
ASENS	Output	Averaged hourly sensitivities. List defined by 'AVG_CONC_SPCS' variable in the run script.	ACONC
SENGRID	Output	Last hour's sensitivity fields to be used as initial conditions for the following time period	CGRID
SENWDEP	Output	Sensitivities of wet deposited species	WETDEP1
SENDDEP	Output	Sensitivities of dry deposited species	DRYDEP
REGIONS	Input	Regional definitions	N/A
EGRIDFILE1	Input	Gridded emissions file 1	N/A
EGRIDFILE2	Input	Gridded emissions file 2	N/A
EGRIDFILEn	Input	Gridded emissions file n	N/A
PT3DFILE1	Input	Inline point source emissions file 1	N/A
PT3DFILE2	Input	Inline point source emissions file 2	N/A
PT3DFILEn	Input	Inline point source emissions file n	N/A
PT3DSTACK1	Input	Inline point source stack groups file 1	N/A
PT3DSTACK2	Input	Inline point source stack groups file 2	N/A
PT3DSTACKn	Input	Inline point source stack groups file n	N/A
BNDY_GASC_S	Input	Sensitivity field boundary conditions	BCON
INIT_GASC_S	Input	Sensitivity field initial conditions	ICON

DDM Applications

- Detecting error apportionment for air quality models (kang et al., 2013)
 - Decomposed concentrations time series to figure out the source of error (emission)
 - Determined the optimum emission perturbation to have the minimum MB in ozone concentration using sensitivity results in DDM
- Determining the source contribution of pollutant concentrations (Itahashi et al., 2013)
 - Studied sensitivity of episodic ozone pollution during 2007 to precursor emissions coming from different sources (China,

Results

- ✓ DDM test runs on: **Aug 2, 2016 at 14:00**
- ✓ Sensitivity unit: **ppb** of ozone per unit change of the parameter (per 1%!)
 - **Positive sensitivity:** Increasing the parameter will **increase** ozone concentration and decreasing the parameter will decrease ozone concentration
 - **Negative sensitivity:** Increasing the parameter will **decrease** ozone concentrations and decreasing the parameter will increase ozone concentration

DDM Test Runs

Ozone sensitivity to total emission of VOC and NOx

Ozone sensitivity to mobile emission of VOC and NOx

Ozone sensitivity to boundary condition of VOC and NOx

Ozone sensitivity to initial condition of VOC and NOx

Ozone sensitivity to Tri-cities regional emission of VOC and NOx

Ozone sensitivity to Spokane regional emission of VOC and NOx

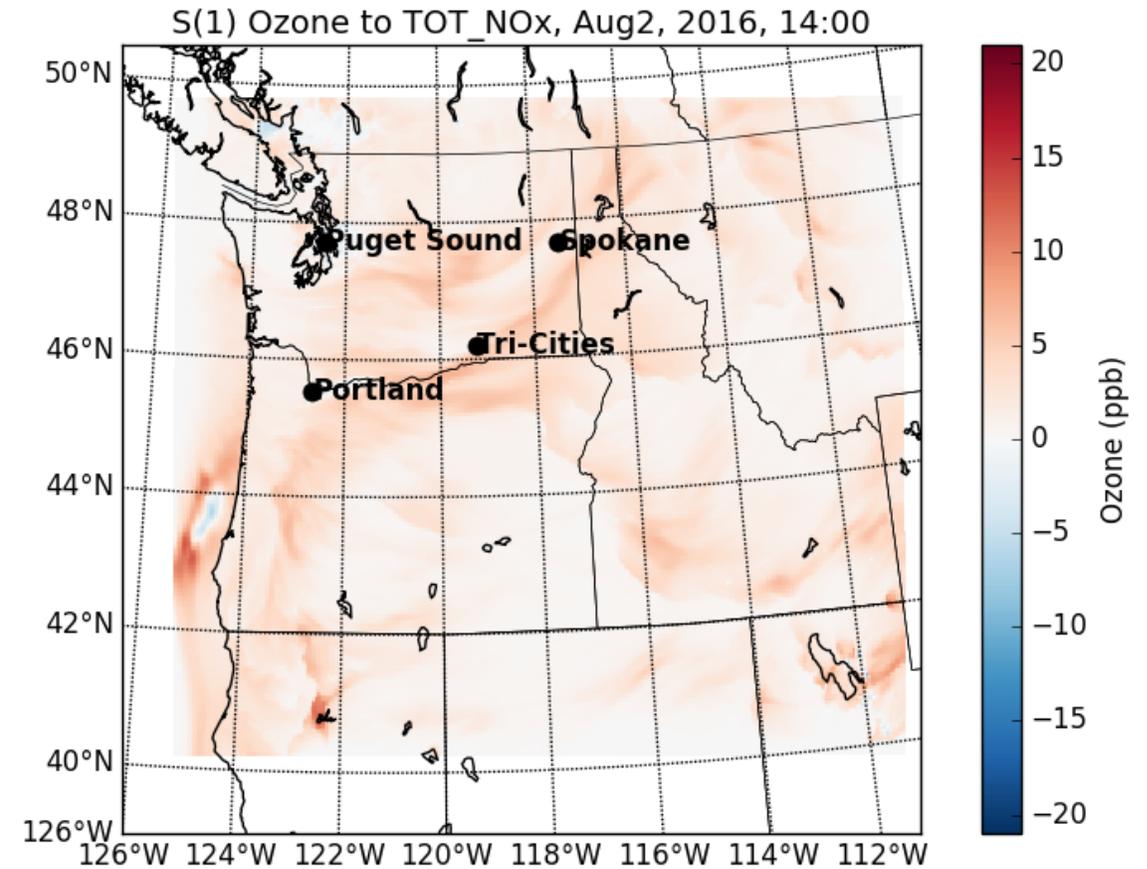
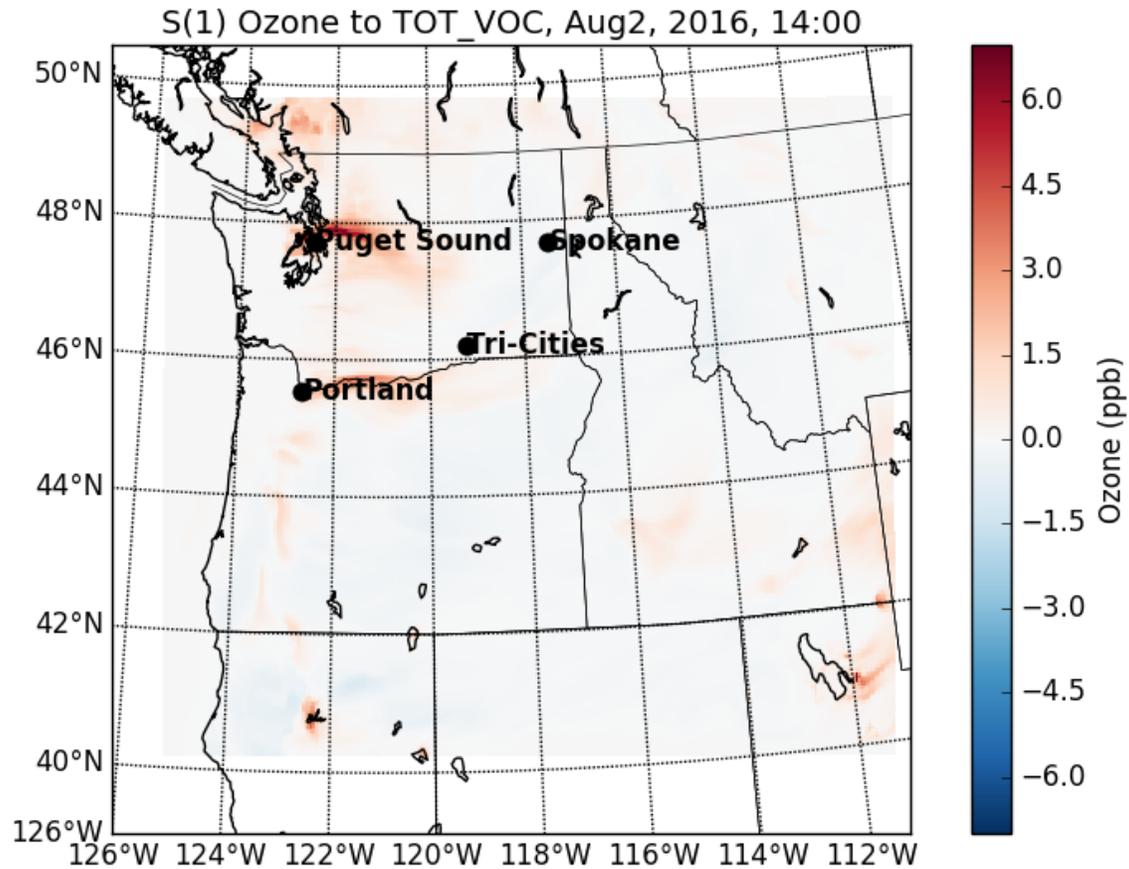
Ozone sensitivity to Puget Sound regional emission of VOC and NOx

Ozone sensitivity to Portland regional emission of VOC and NOx

Ozone Sensitivity to Total Emissions of NOx and VOC

O3 sensitivity to VOC range: -1.1564 to 6.9137 ppb

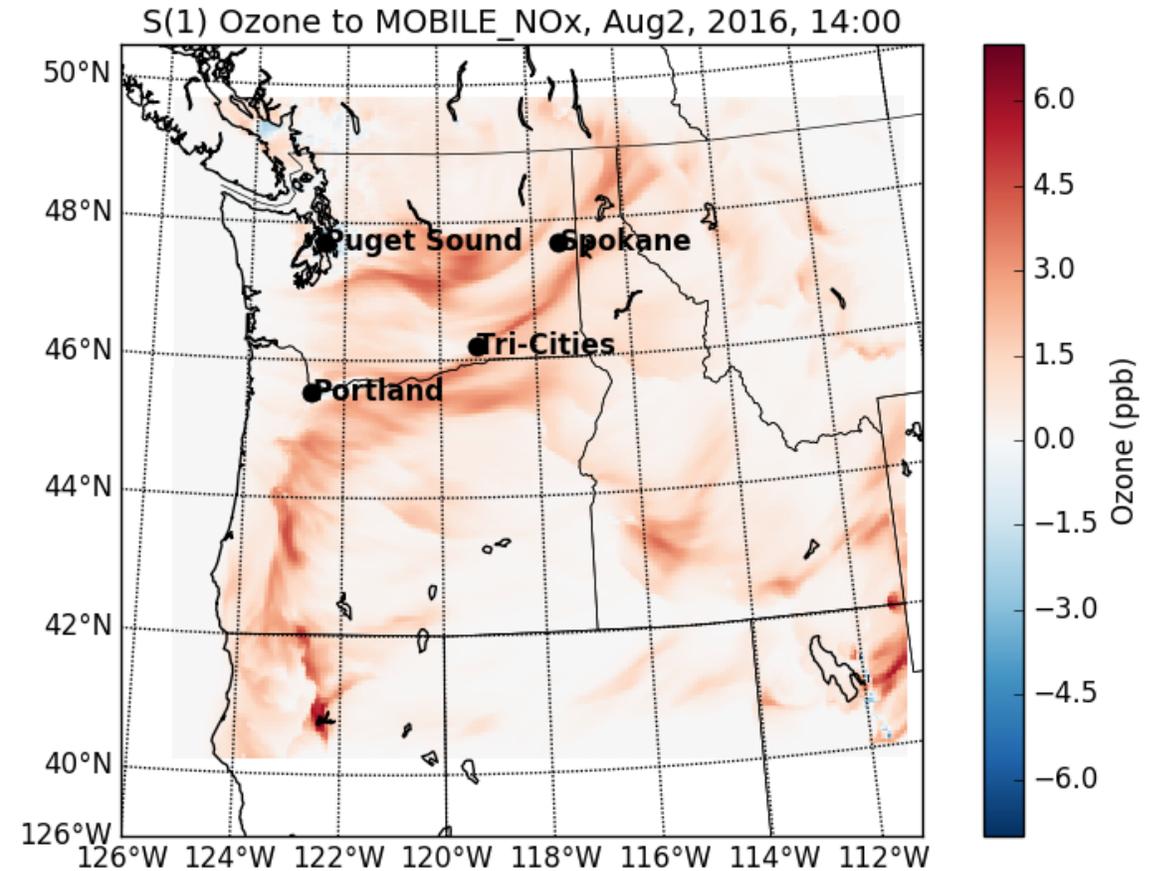
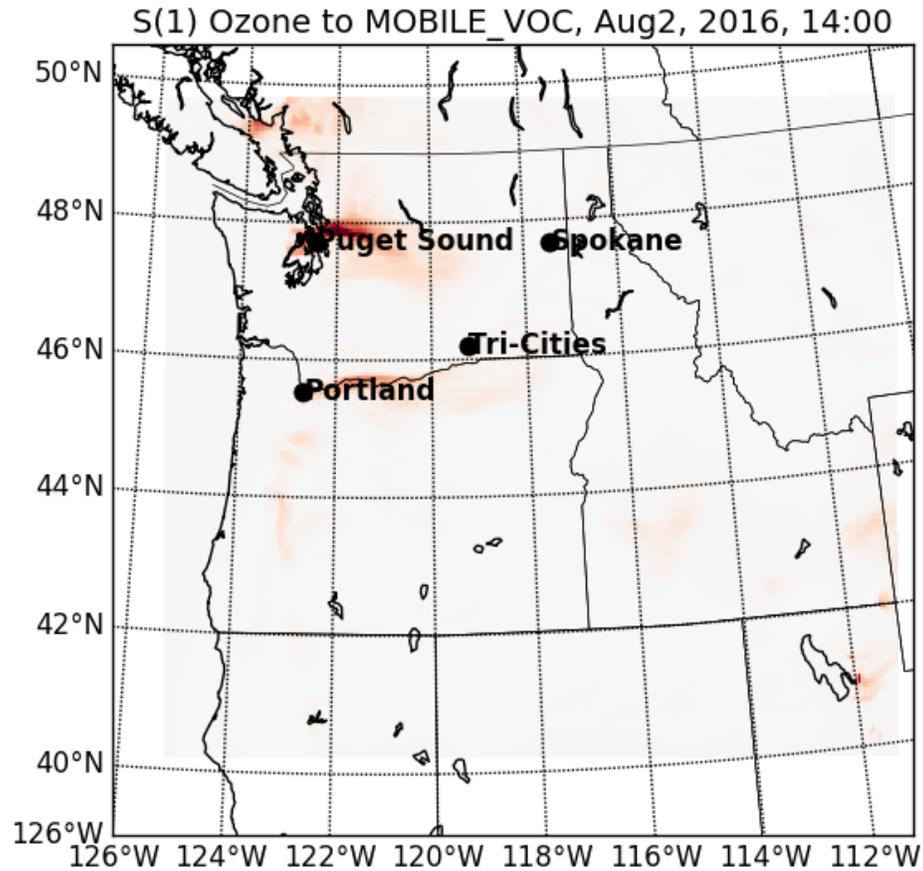
O3 sensitivity to NOx range: -20.7507 to 12.8291 ppb



Ozone Sensitivity to Mobile Emissions of NOx and VOC

O3 sensitivity to VOC range: -0.02176 to 1.4378 ppb

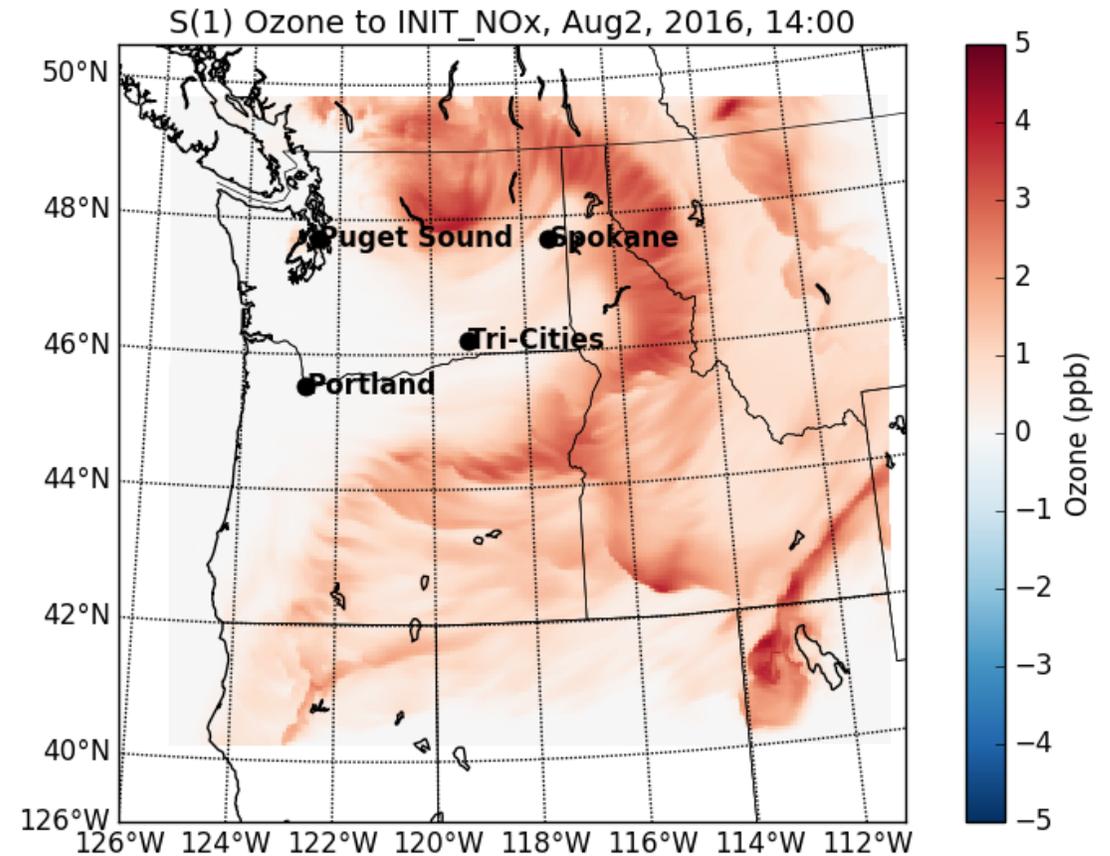
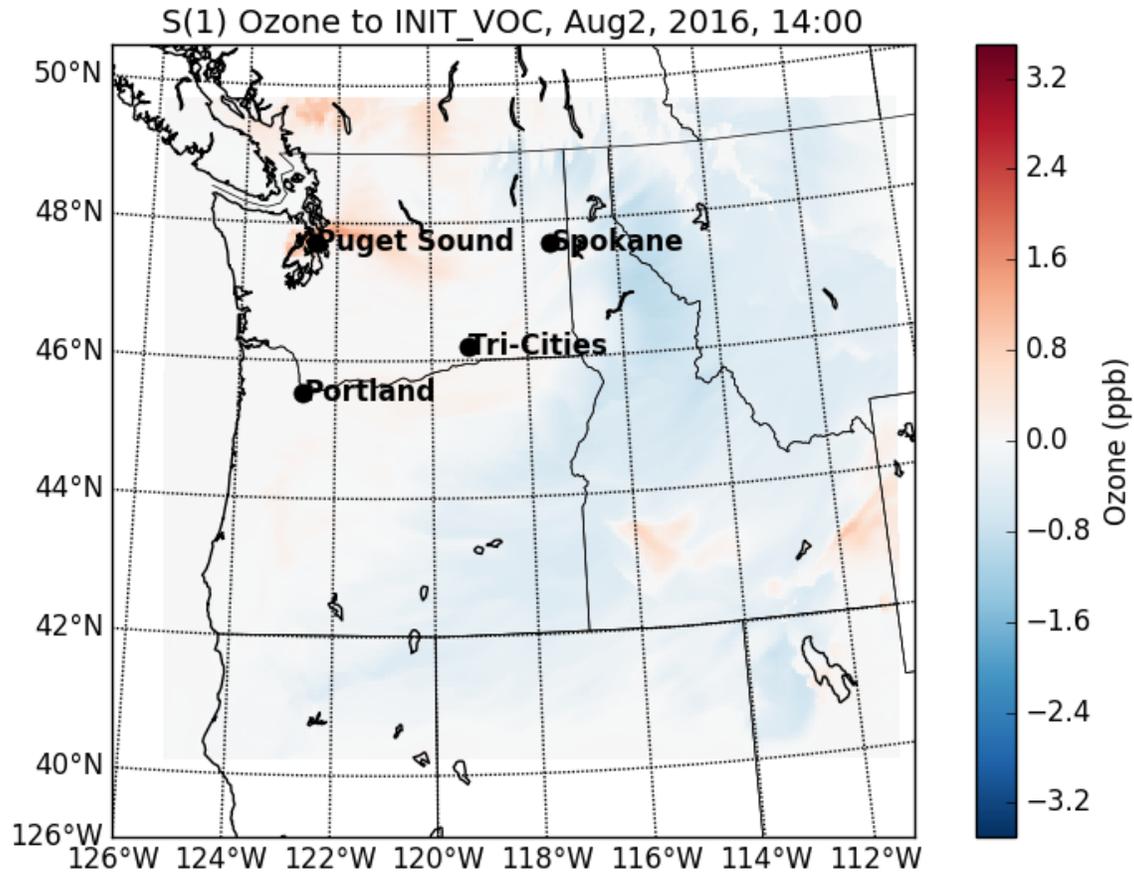
O3 sensitivity NOx range: -6.9253 to 5.3875 ppb



Ozone Sensitivity to Initial Conditions of NOx and VOC

O3 sensitivity to VOC range: -0.9852 to 3.4972 ppb

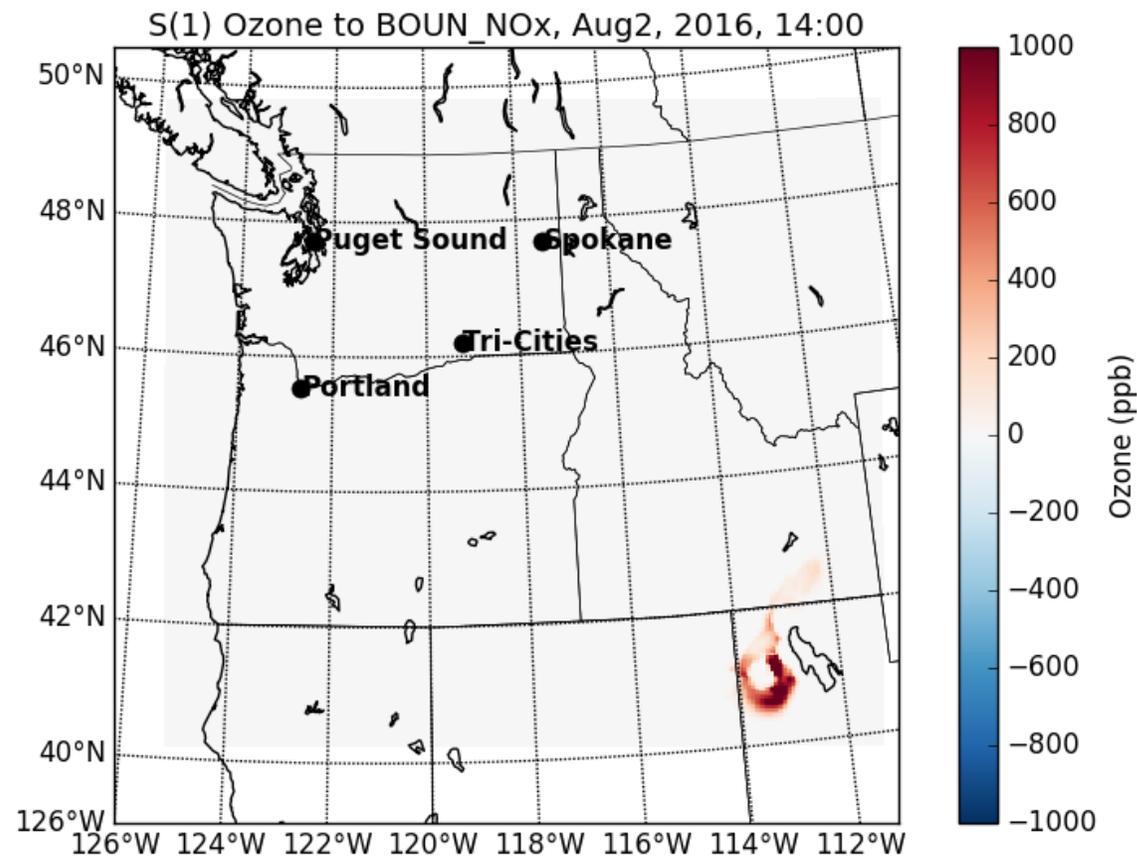
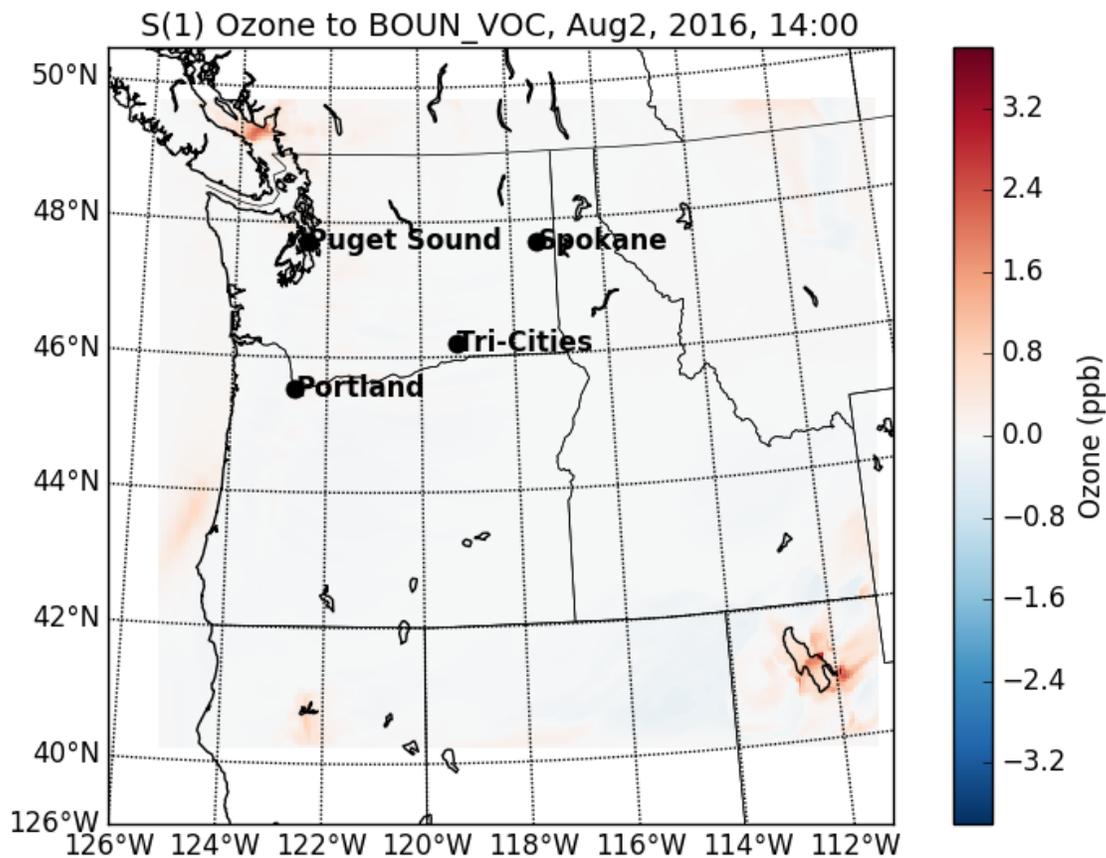
O3 sensitivity NOx range: -0.9406 to 4.8300 ppb



Ozone Sensitivity to Boundary Conditions of NOx and VOC

O3 sensitivity to VOC range: -0.3023 to 3.6192 ppb

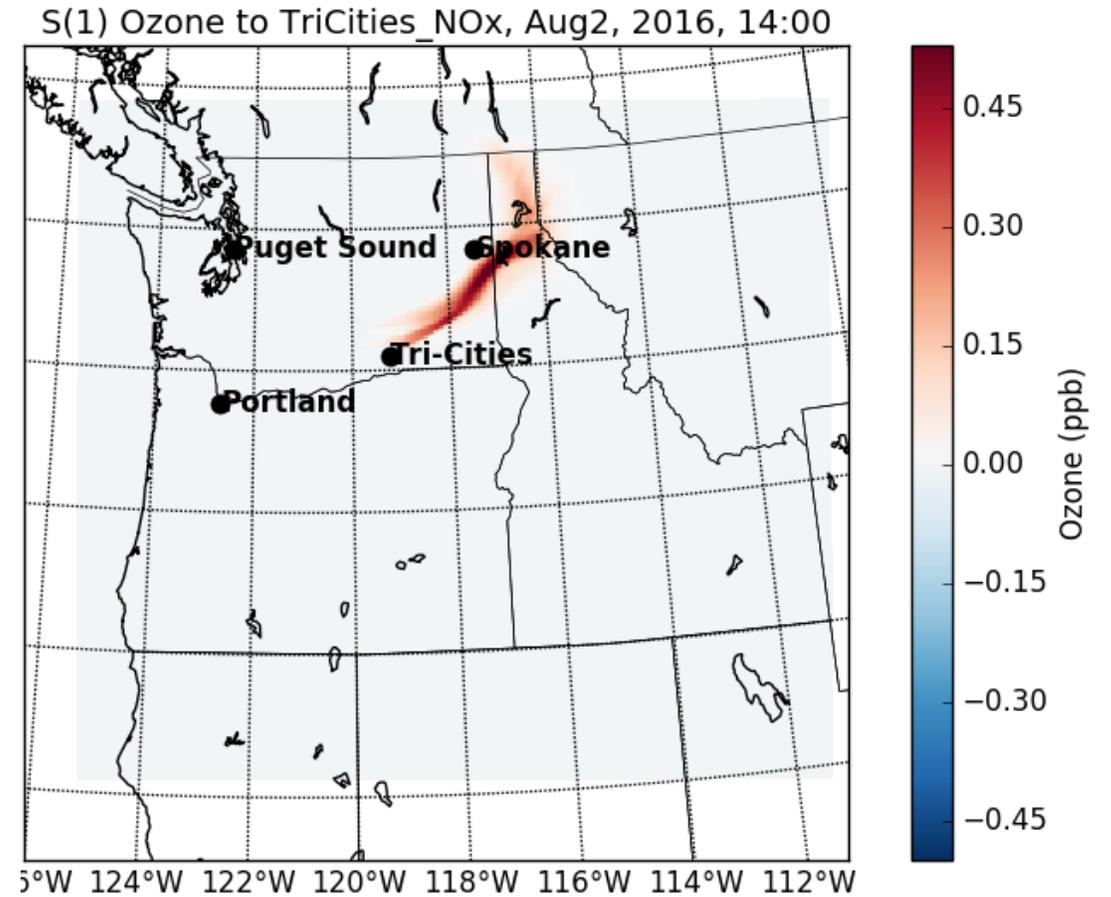
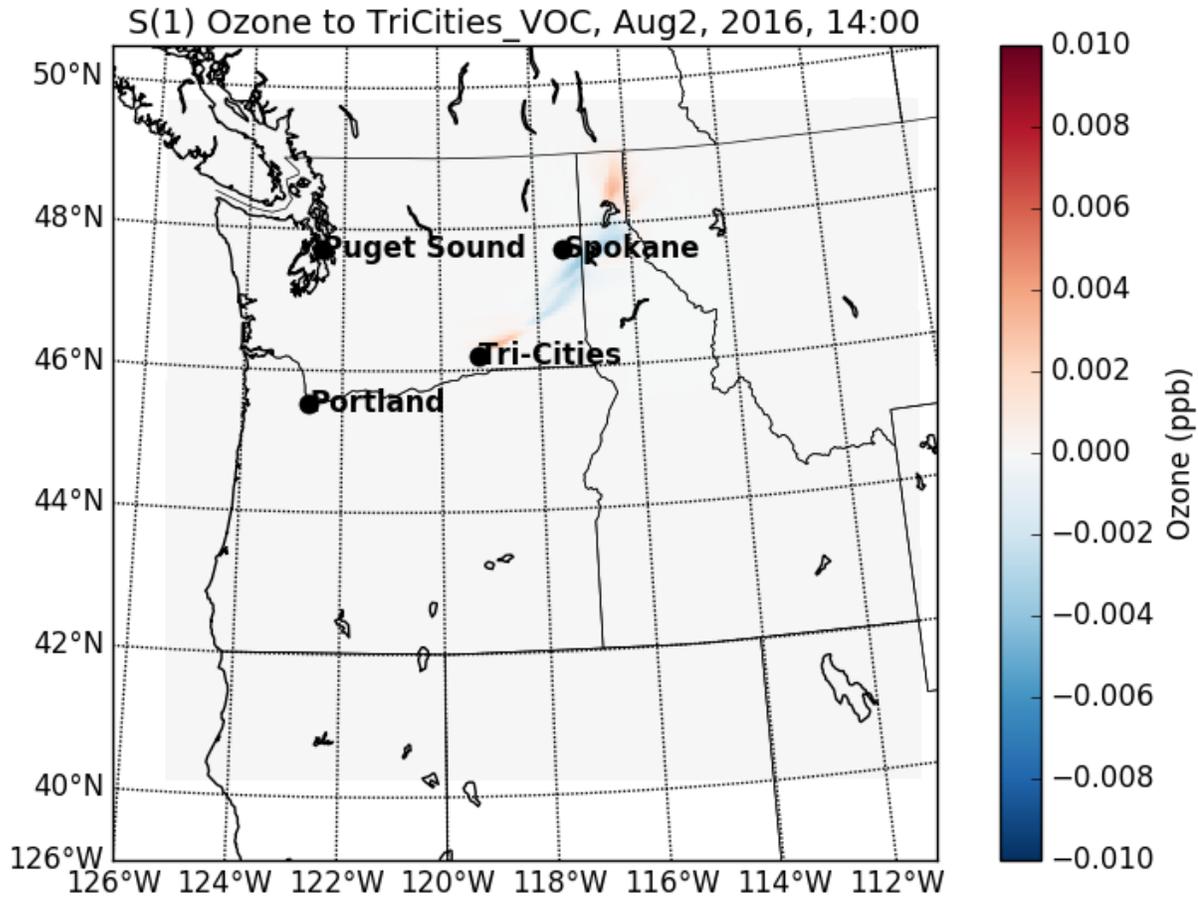
O3 sensitivity NOx range: -0.3606 to **4547** ppb



Ozone Sensitivity to Tri-Cities Mobile Emissions of NOx and VOC

O3 sensitivity to VOC range: -0.0024 to 0.0179 ppb

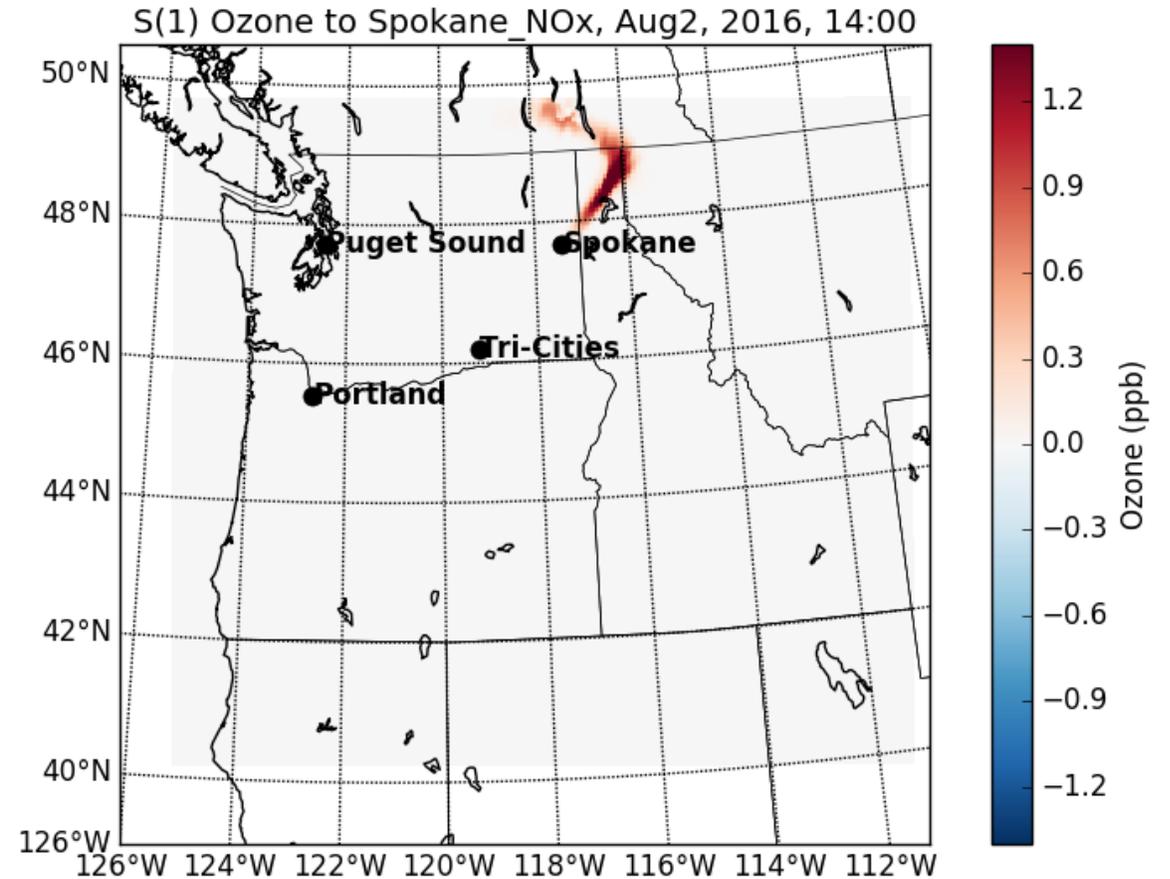
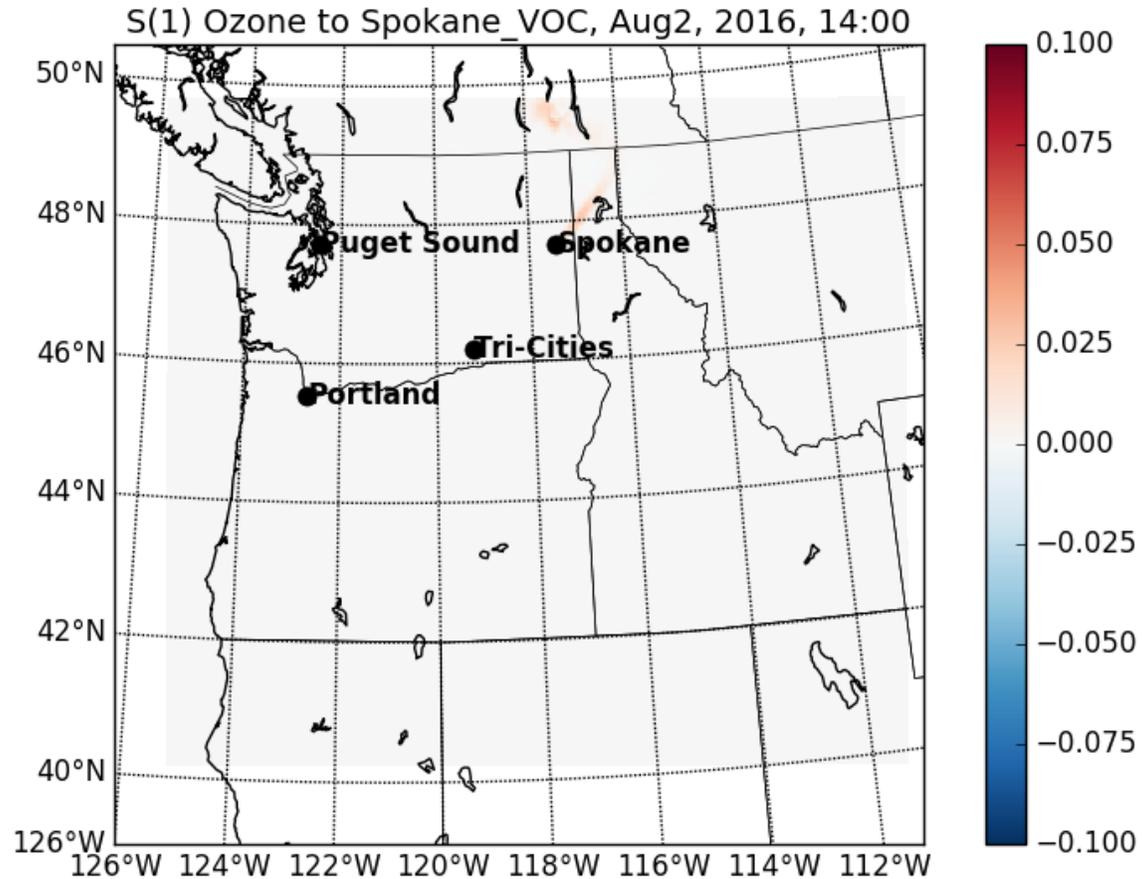
O3 sensitivity NOx range: -0.4889 to 0.5249 ppb



Ozone Sensitivity to Spokane Mobile Emissions of NOx and VOC

O3 sensitivity to VOC range: -0.000964 to 0.1317 ppb

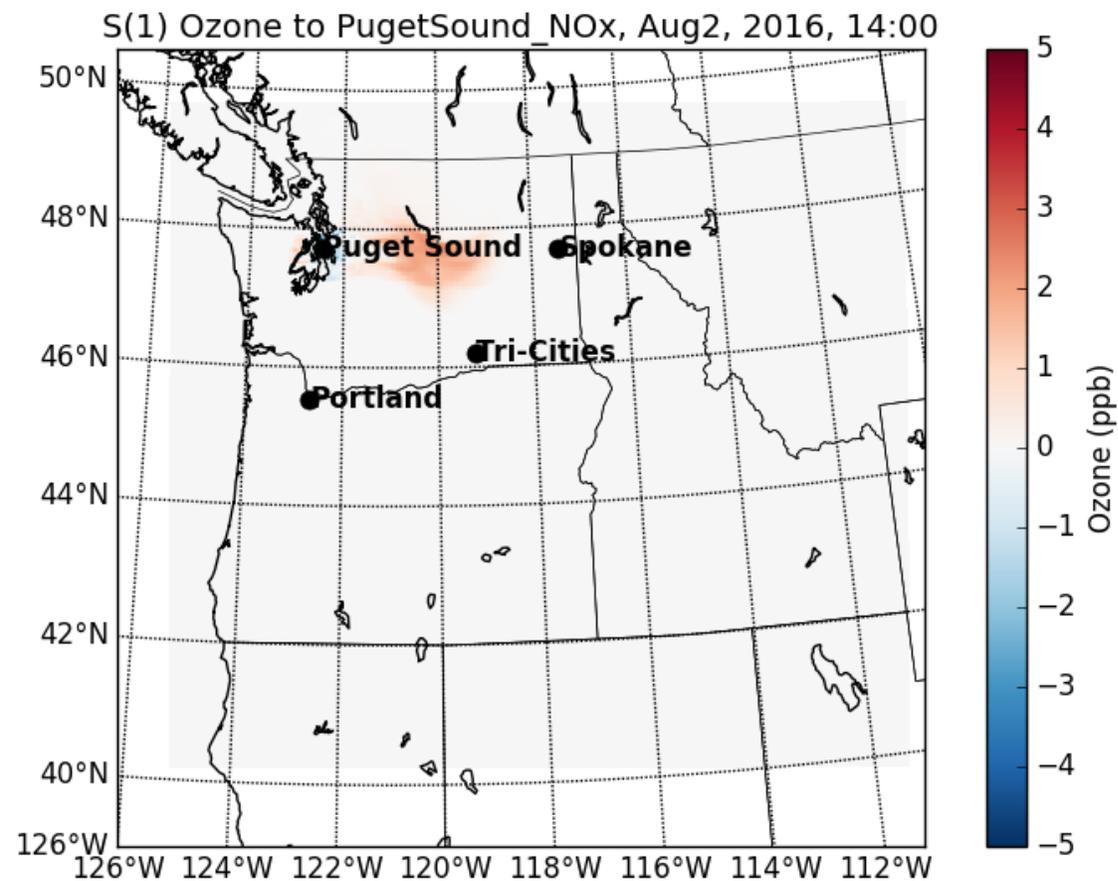
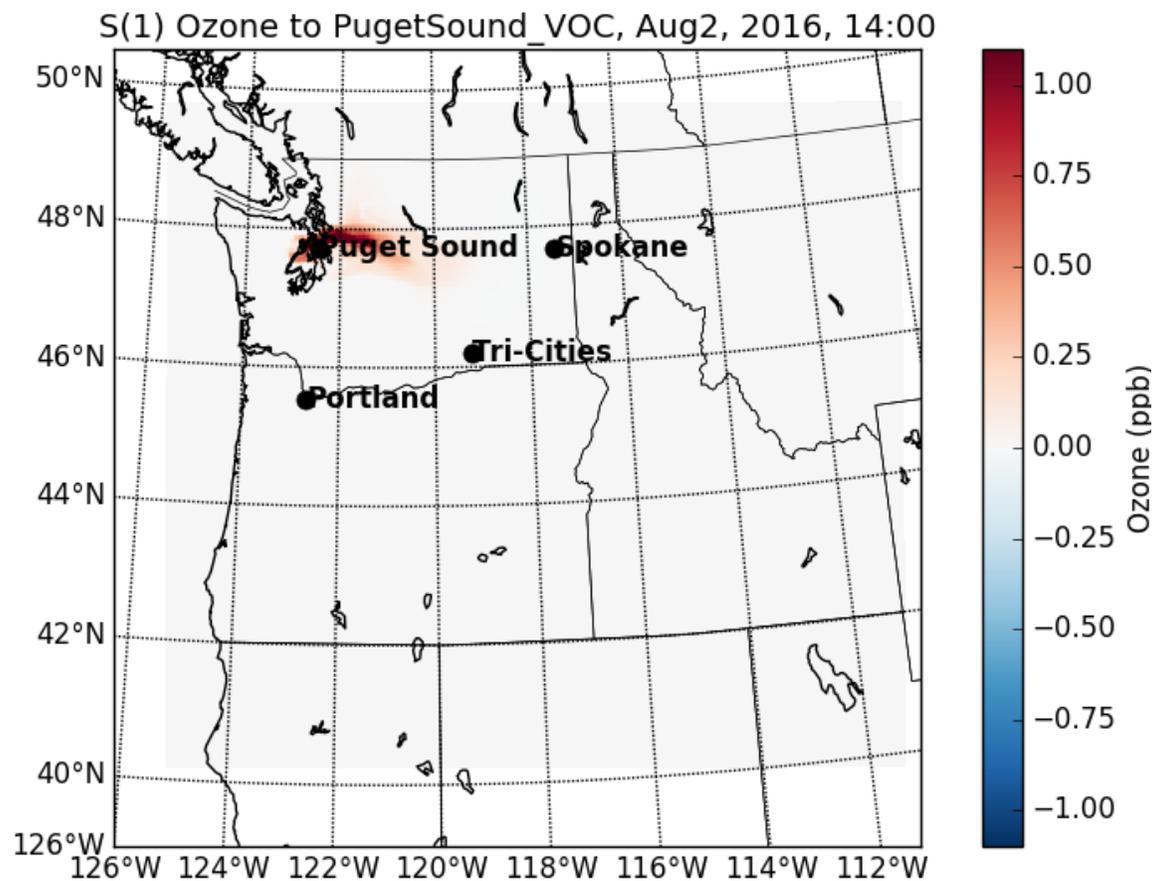
O3 sensitivity NOx range: -1.3077 to 1.2805 ppb



Ozone Sensitivity to Puget Sound Mobile Emissions of NOx and VOC

O3 sensitivity to VOC range: -0.0000137 to 1.0851 ppb

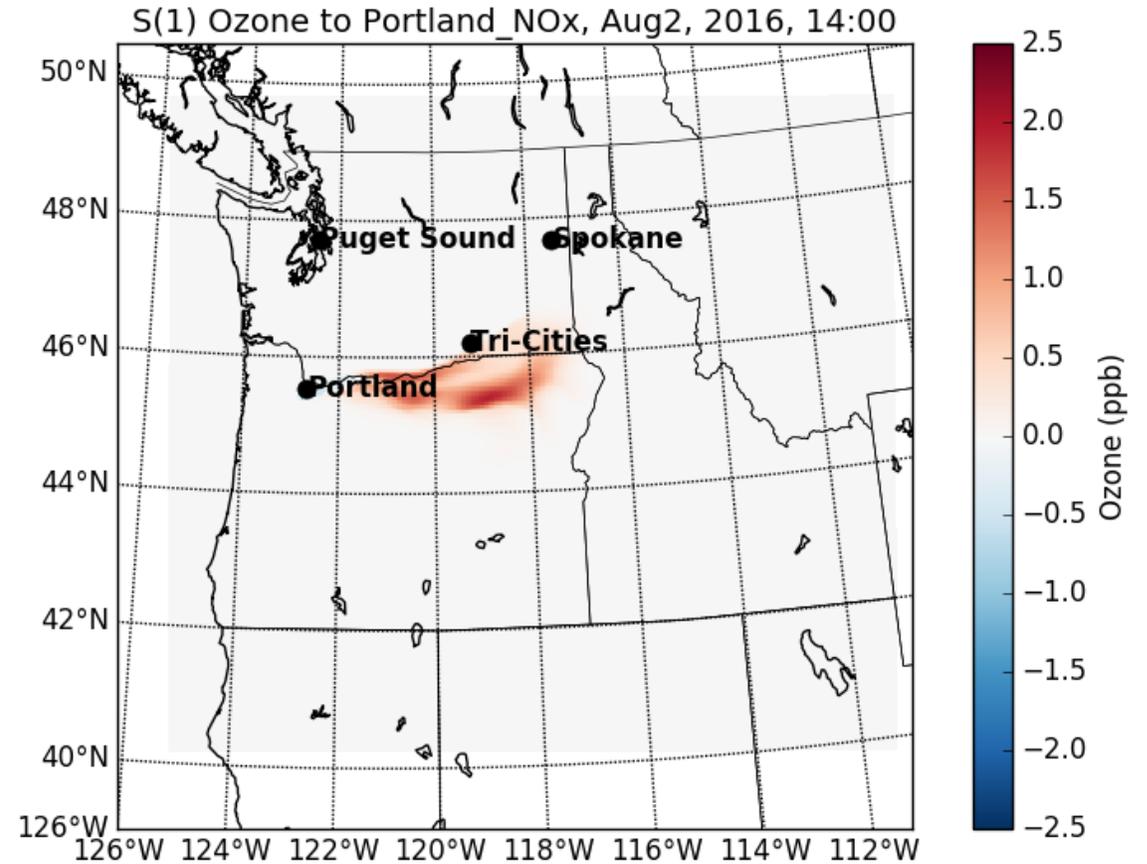
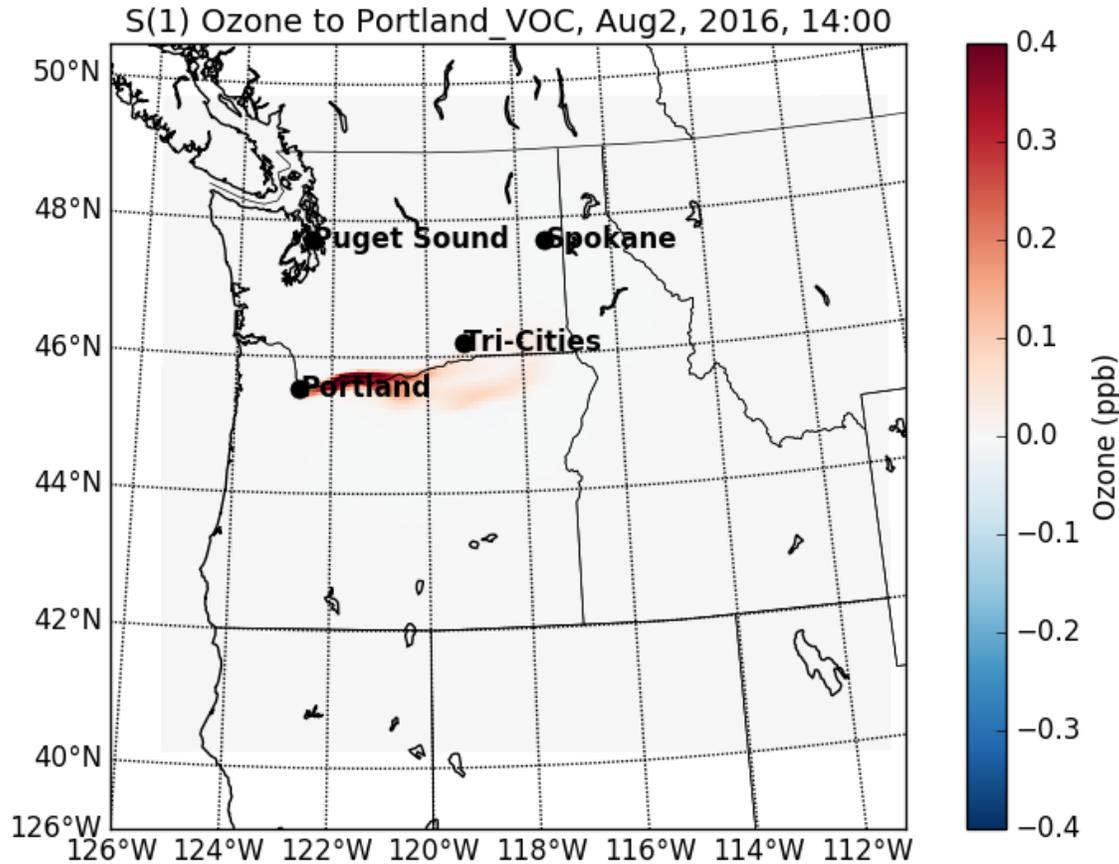
O3 sensitivity NOx range: -4.0586 to 2.3851 ppb



Ozone Sensitivity to Portland Mobile Emissions of NOx and VOC

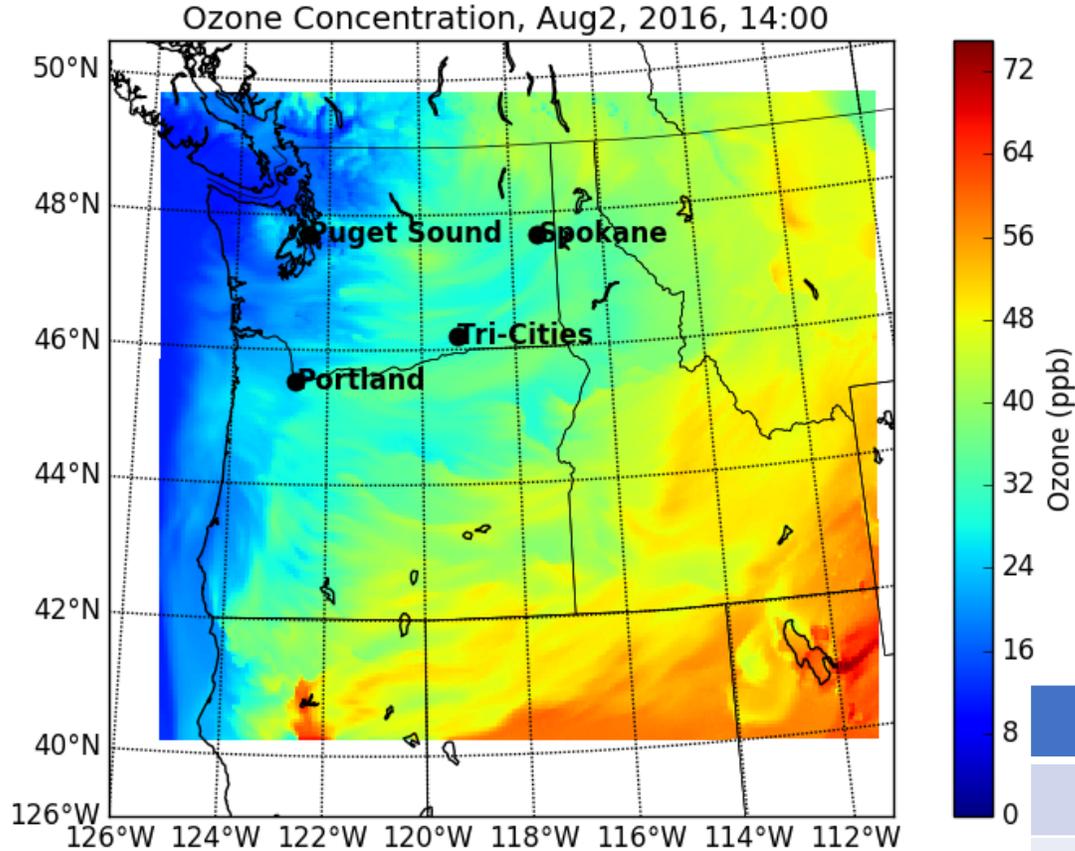
O3 sensitivity to VOC range: -0.00311 to 0.40719 ppb

O3 sensitivity NOx range: -2.5710 to 1.1769 ppb



Conclusions

Ozone concentration range: 0.0 to 73 ppb



- Regions with low sensitivity seems to generate ozone so efficiently
- Small sensitivities make it harder to control ozone concentration

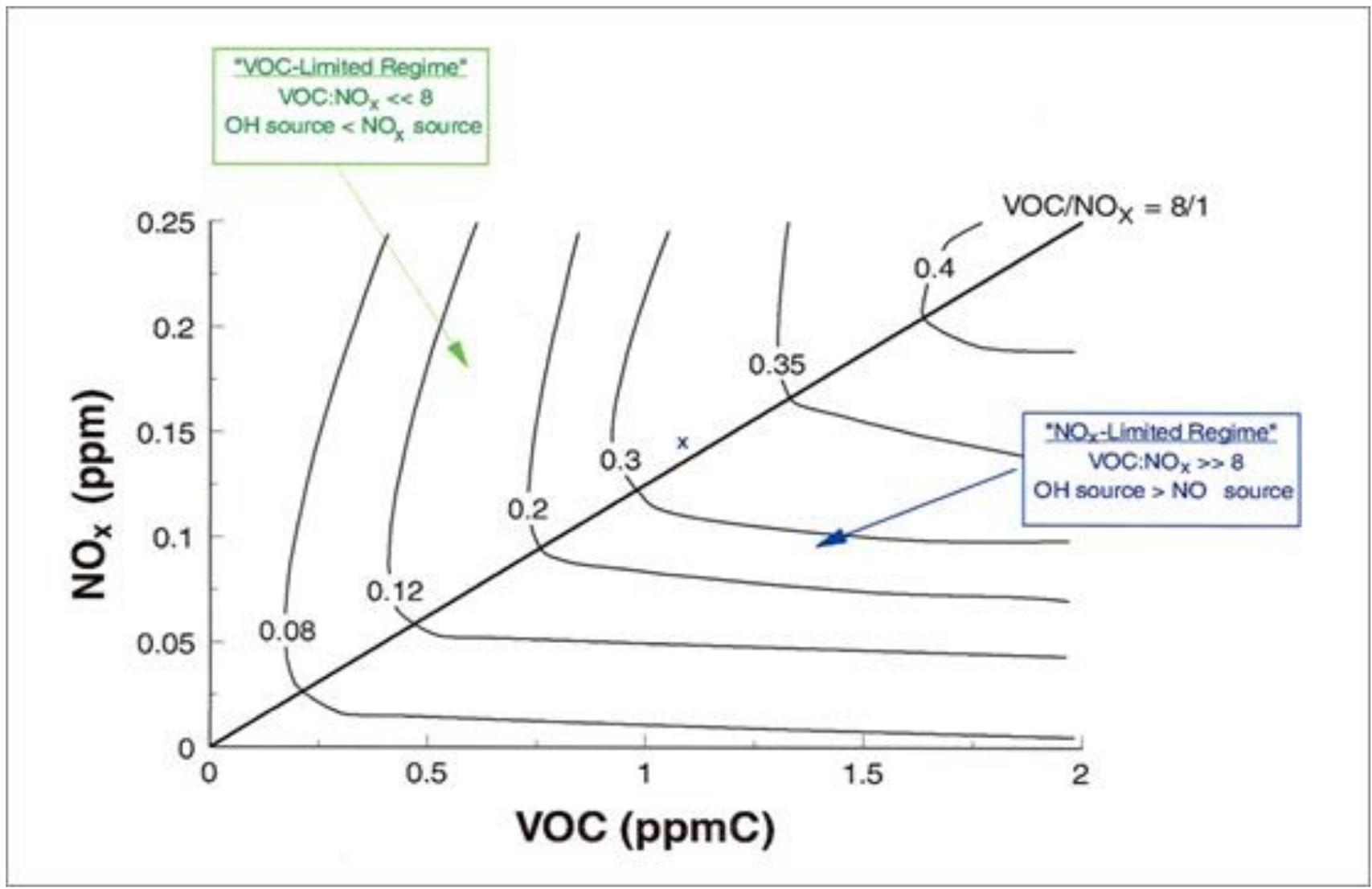
	Ozone Sensitivity to VOCs		Ozone Sensitivity to NOx	
	min	max	min	max
Tri-cities	-0.0024	0.0179	-0.4889	0.5249
Spokane	-0.000964	0.1317	1.3077	1.2805
Puget Sound	-0.0000137	1.0851	-4.0586	2.3851
Portland	-0.00311	0.40719	-2.5710	1.1769

Future work

- Test the outputs by running CMAQ using the brute force method
- Comparing sensitivity coefficient calculated using DDM with the ones calculated using indicator ratios (experimental method)
- Run the model to calculate second and higher order sensitivity

Thank you

Questions/Discussions?



DDM Control file example

```
EMISSO2
  EMIS
    GRID
    1
    EGRIDFILE1
    PT3D
    2
    PT3DSTACK1
    PT3DFILE1
    PT3DSTACK2
    PT3DFILE2
  SPECIES
  SO2

EMISNOX
  EMIS
  SPECIES
  NO
  NO2

2ENOX
  HIGH
  EMISNOX
  EMISNOX
```