

# Assessing Influences of Ozone Precursor Emissions on Human Health and Ecosystems

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## I. Motivation

The Clean Air Act supports the establishment of a national standard for ambient concentrations of atmospheric pollutants to protect human health and public welfare (CAA, 1990). The primary standard has been viewed as sufficient for also protecting public welfare. We seek to explore how emissions affect these regulatory endpoints differently in the CMAQ chemical transport modeling framework.

### Distinct spatial distributions

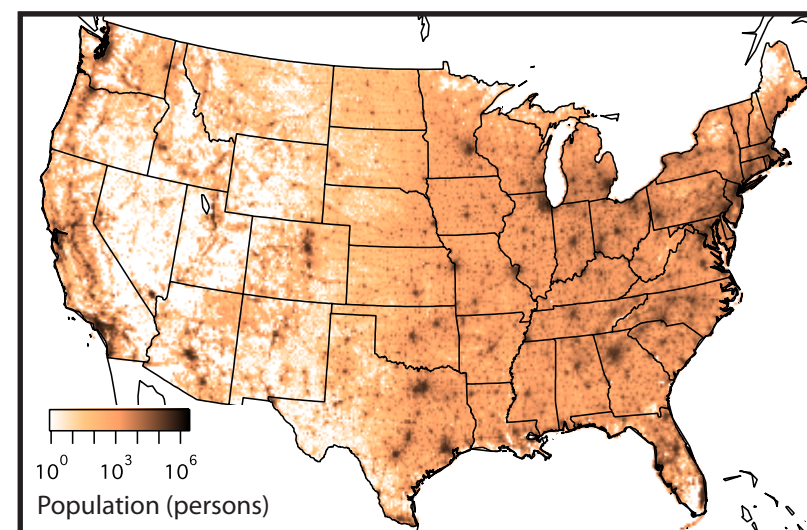


Figure 1. Gridded human population in 2010

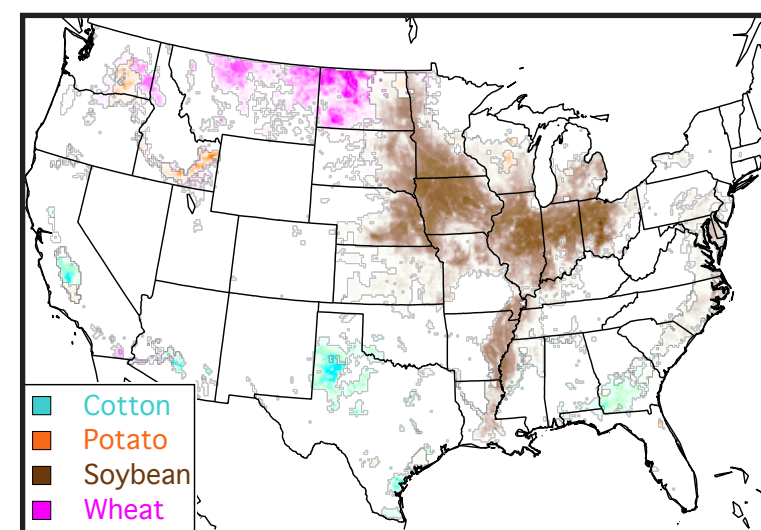


Figure 2. Gridded crop production in 2007.

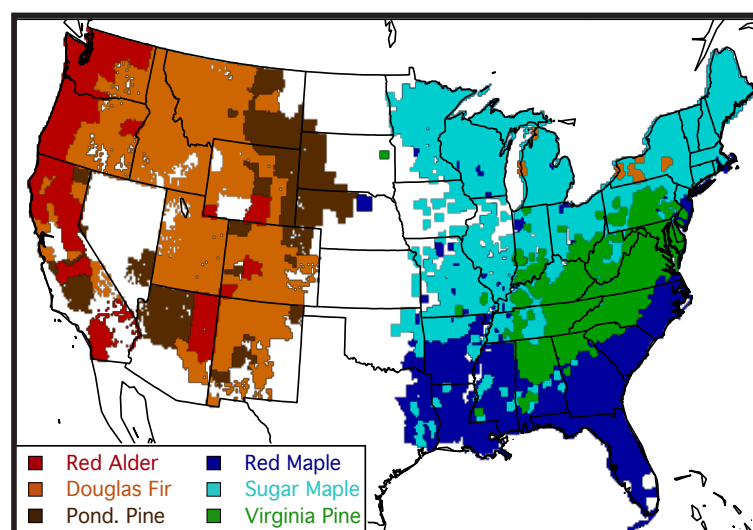


Figure 3. Gridded presence of tree species.

Generally, dense human populations are located separately from sensitive ecosystems. Urban non-attainment areas often contain vegetation, but the majority of crops and timber are located in more rural areas where ozone monitors may be more scarce. The separation of these vulnerable populations in space allows the possibility that emissions influences on each endpoint are unique.

### Unique response regimes

Epidemiological studies have revealed association between peak ozone concentrations and increased mortality rates (Bell et al., 2004; Schwartz, 2005; Jerrett et al., 2009); therefore, reducing peak ozone concentrations has been the focus of the primary standard, which is formulated as a limit on the 4th highest daily maximum 8-hr average ozone concentration. Over the last three decades, a 25% reduction in this metric has been achieved nationally.

Plants also demonstrate reduced productivity when exposed to elevated ozone concentrations (e.g., Lesser et al., 1990, Mills et al., 2007). However, cumulative exposures to lower concentrations have been shown to reduce yield of crops (and decrease the biomass production of trees (EPA REA, 2012)). In addition to responses varying with ozone concentration, the water vapor concentration, to which stomata respond, also affects the influence of ozone on plant health.

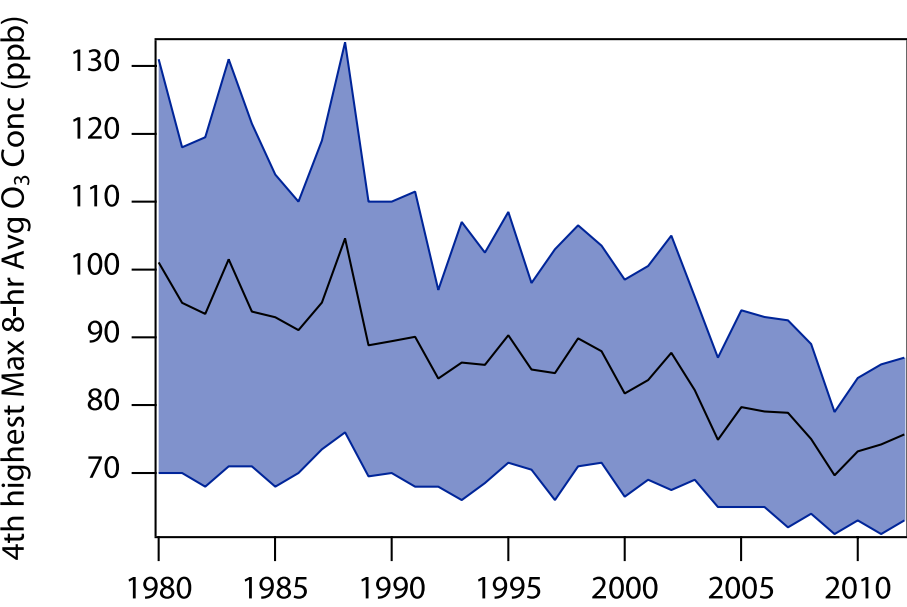
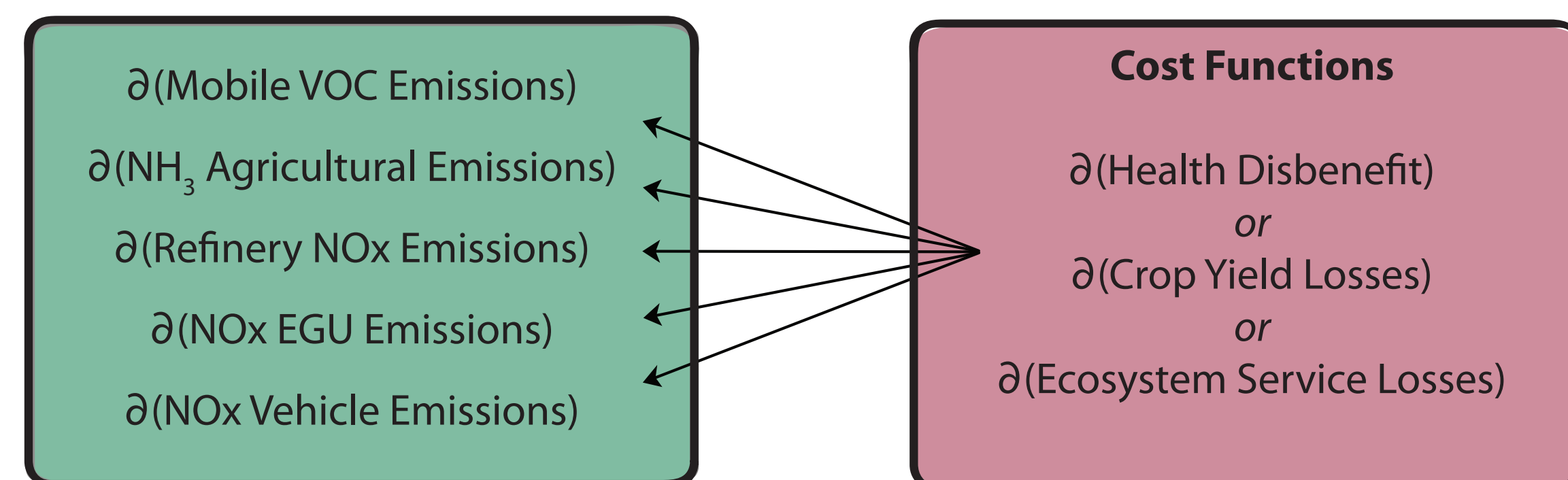


Figure 4. 4th greatest maximum 8-hr average monitored O<sub>3</sub> concentrations have declined over past decades due to emissions controls.

Although further refinement of and mechanistic explanations for each dose-response relationship are active areas of research in both human and plant populations, current understanding reveals that both cumulative, lower-concentration and acute, higher-concentration ozone exposure can degrade human health and public welfare. Thus, the relative roles of emissions sources in each endpoint may very well be distinct, potentially warranting consideration of unique regulatory treatment.

## II. CMAQ adjoint framework

$$\partial x = (F')^T(x, \partial J)$$



The CMAQ adjoint framework of Hakami et al., (2007) facilitates the assessment of relative contributions of each modeled emissions source with respect to a concentration-based metric. Specifically, the derivative of the mathematical relationship between emissions and concentrations is established by the adjoint model. The model adjoint ingests an adjoint forcing, which is a concentration-based metric of interest (i.e., estimated mortality due to chronic ozone exposure). The result of the adjoint calculation is an efficient determination of the relative influence of each emissions parameter on the cost function, even with thousands of parameters.

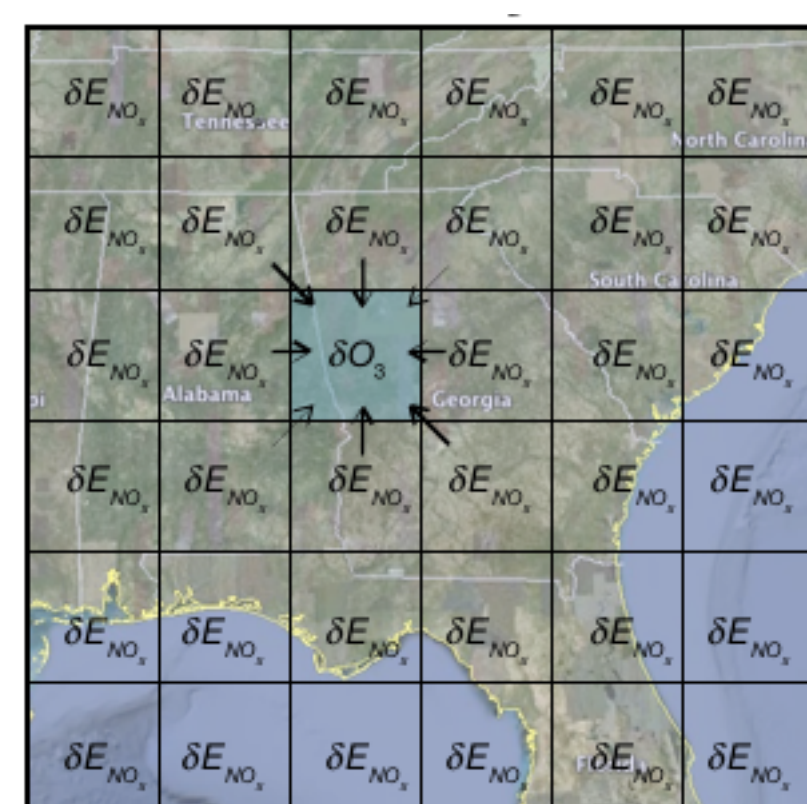


Figure 6. Depiction of the spatial specificity of adjoint sensitivities provide when relating the influence of emissions on concentration-based metrics.

When applied, the CMAQ adjoint transforms the adjoint forcing through the chemical and physical processes in the same manner as the forward model treats emitted species. In order to use the CMAQ adjoint to assess the influence of emissions on distinct regulatory endpoints, we must define the cost functions that represent the degradation caused by ozone exposure. Here, we discuss the formulation of human health and ecological cost functions based on 2007 modeled ozone concentrations and vulnerable species distributions. One can consider adjoint forcing functions as input to the adjoint model; by analogy to the forward modeling framework, the spatial and temporal resolution is similar to emissions.

## III. Evaluating Degradation of Human Health

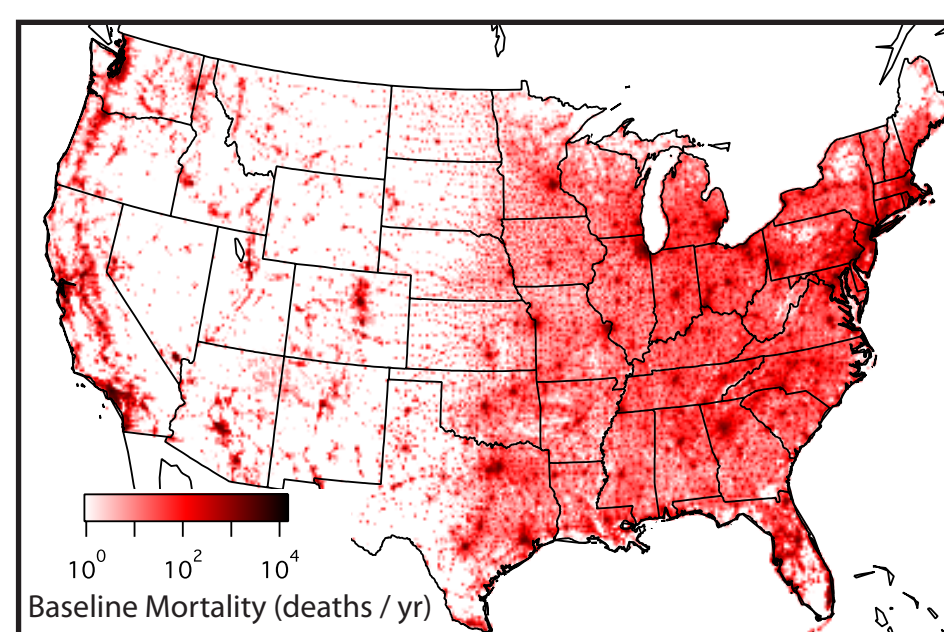


Figure 7. Baseline mortality rate.

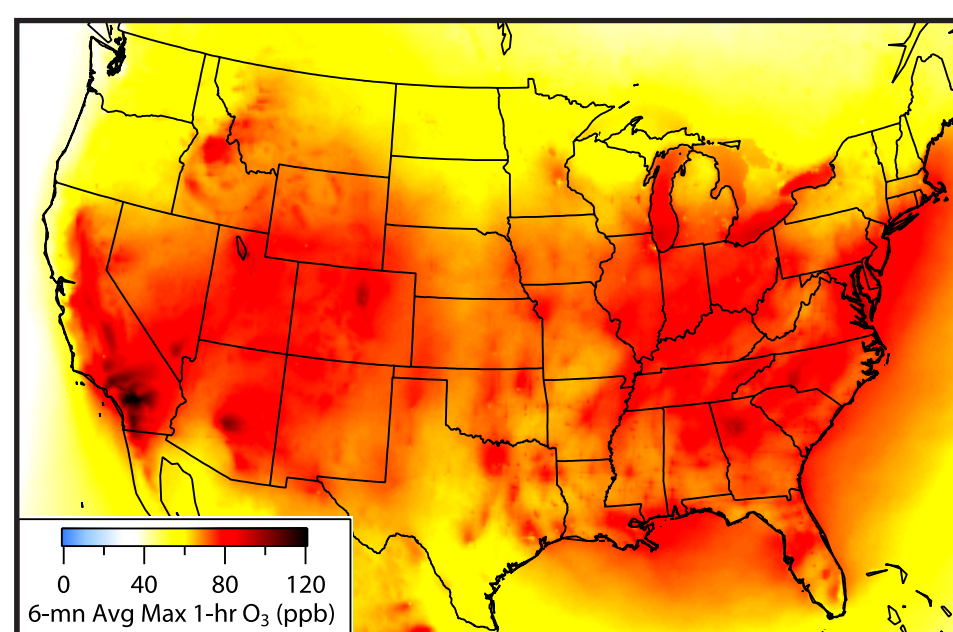


Figure 8. Six-month average maximum hourly ozone concentration based on CMAQ model output for 2007. years of age.

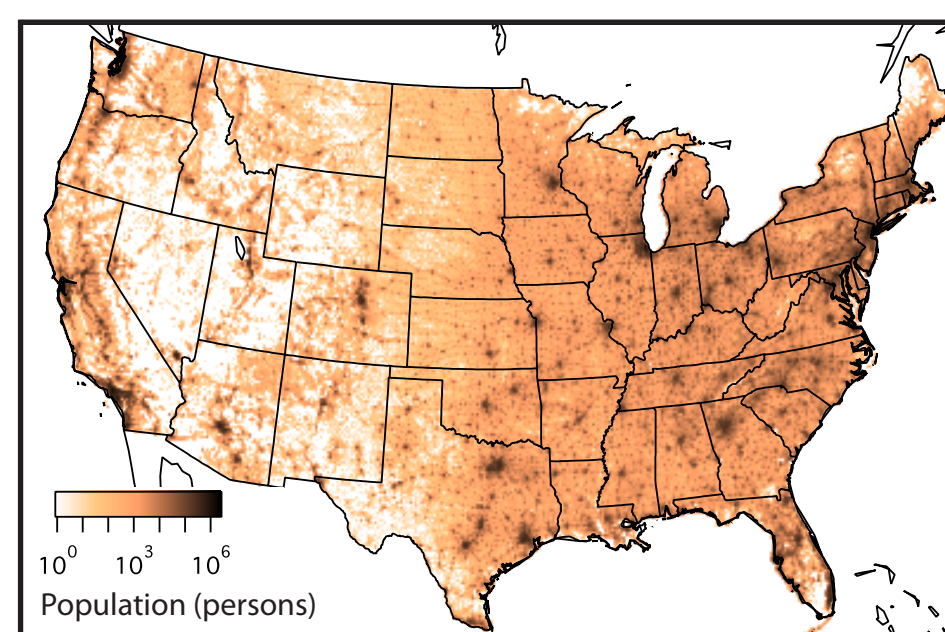


Figure 9. Distribution of human population above 30 concentration based on CMAQ model output for 2007. years of age.

Recent work by Jerrett et al. (2009) has associated long-term exposure to ozone with death from respiratory causes. The following equation provides a relationship between modeled ozone concentrations and increased mortality rates.

$$\frac{\partial(\text{Mortality})}{\partial(\text{Conc}_i)} = M_0 \text{Pop}_{(>30)} \beta(\exp[-\beta \text{Conc}_i])$$

where  $M_0$  represents the baseline mortality rate in each grid cell (Fig. 7).  $\text{Conc}_i$  is the six-month mean of the hourly maximum concentration of ozone in each grid cell (Fig. 8).  $\text{Pop}_{(>30)}$  represents the humans in each grid cell above 30 years of age (Fig. 9).  $\beta$  is a coefficient determined in the study (0.04 increased mortalities due to respiratory illness per 10 ppb increase in ozone metric) (Jerrett et al., 2009). The offline manner of calculating the adjoint forcing function is particularly useful in this and similar cases where the variable of interest is a function of concentration over a long period of time.

To assess the relative contribution of emissions throughout the episode to the mortality associated with long-term ozone exposure, we prepare an adjoint forcing array that spans the spatial and temporal extent of the modeled domain. Similar to the method of Pappin et al. (2013), we distribute the forcing,  $\partial J$ , in a manner commensurate with the mortality calculation.

$$\frac{\partial(J)}{\partial([O_3])} = \left[ \frac{\partial(\text{Mortality})}{\partial(\text{Conc}_i)} \right]_{\text{max 1-hr } [O_3]}$$

### Mortality-based Adjoint Forcing

June-July-August average

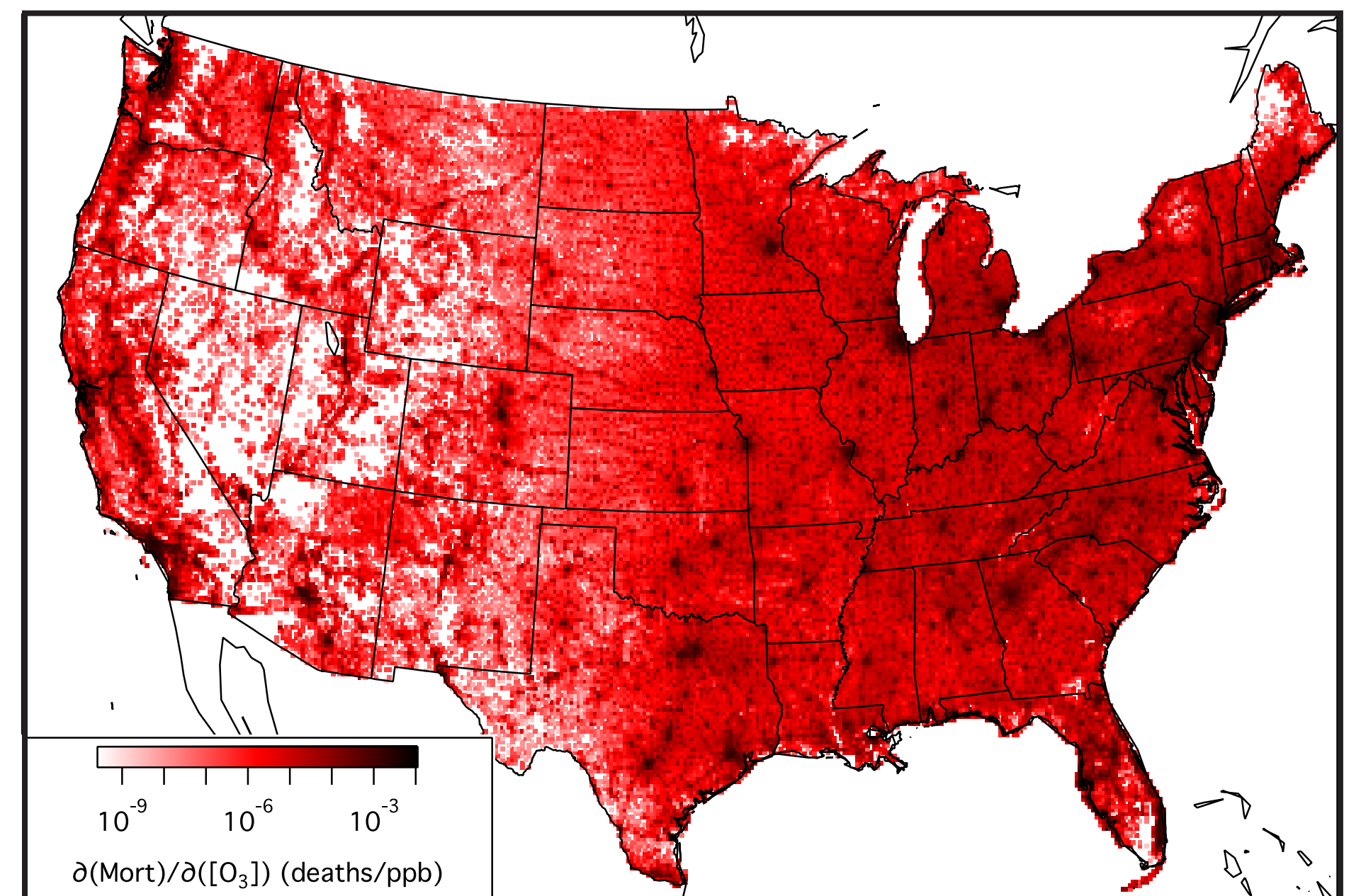


Figure 10. The adjoint forcing function attributes the increased mortality throughout the episode to each grid cell. The forcing is non-zero only in the hour during which the maximum ozone concentration for the day occurs. Here, the average in time of all the non-zero values is shown.

## IV. Assessing Influence on Ecosystems

In a manner similar to human exposure-response calculations, we consider the effect of ozone exposure on crop production. Although a number of different ozone metrics exist that are relevant to ecosystem health, the cumulative peak-weighted index, W126, is the most widely accepted metric in the U.S. The seasonal value is calculated as follows:

$$W126_{90 \text{ day}} = \sum_{i=1}^{90} \left( \frac{[O_3]}{1 + (4403e^{-126[O_3]})} \right)_{i, 8\text{am}-8\text{pm (LST)}} \quad RYL = 1 - \exp \left[ - \left( \frac{W126}{A_i} \right)^{B_i} \right]$$

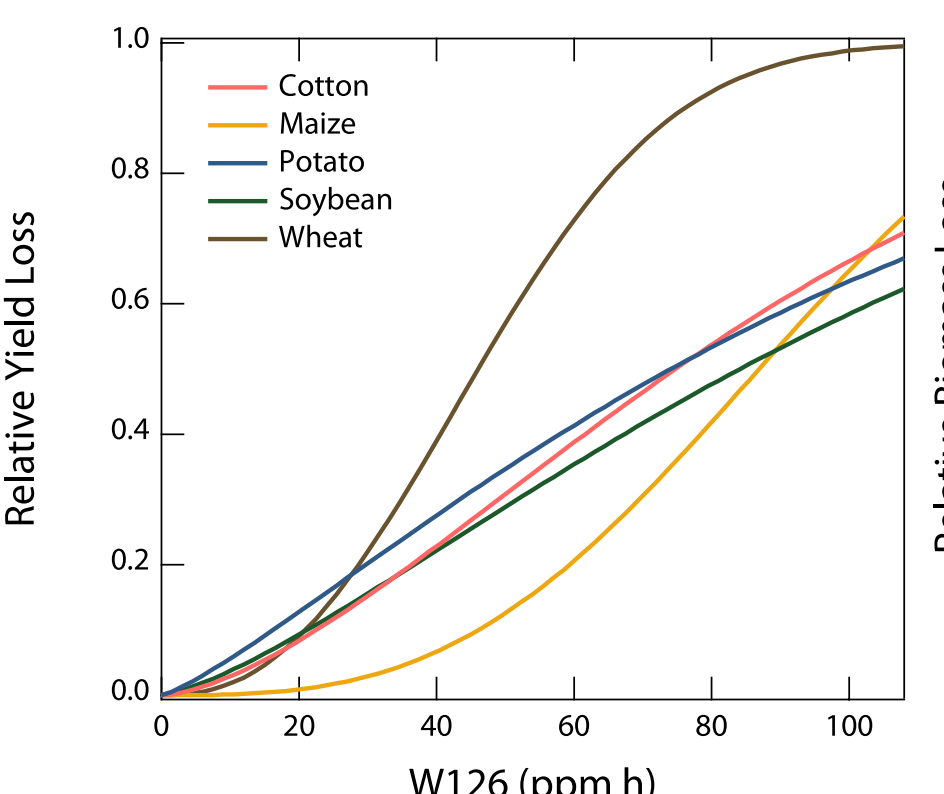


Figure 11. Estimates of the relative yield loss due to cumulative exposure of crops over the summer months.

In laboratory and field studies, exposure to different W126 values has been correlated with loss of yield in a variety of plants and trees. The relative yield loss to W126 relationships are shown for crops (Fig. 11) and timber (Fig. 12). The following equation defines the relationship between the ozone metric W126 and relative yield loss (RYL), where  $A_i$  and  $B_i$  are crop or timber-specific parameters that are empirically determined (Lehrer et al., 2007).

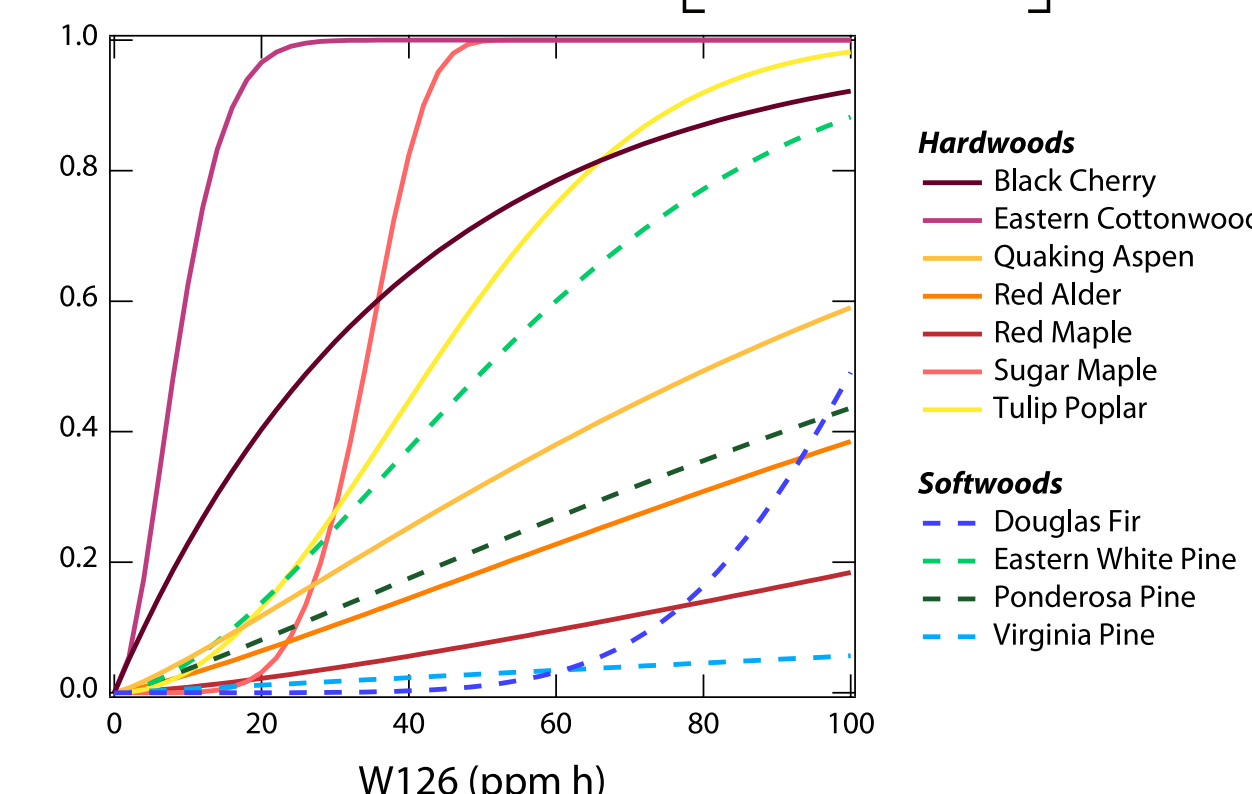


Figure 12. Estimates of the relative biomass loss due to cumulative exposure of trees over the summer months. Softwoods and hardwoods alike can be affected.

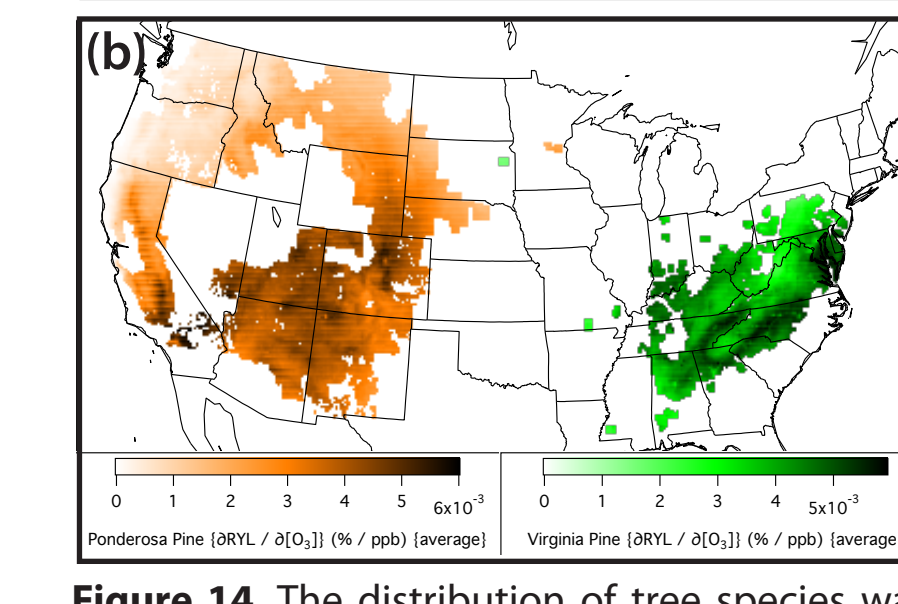
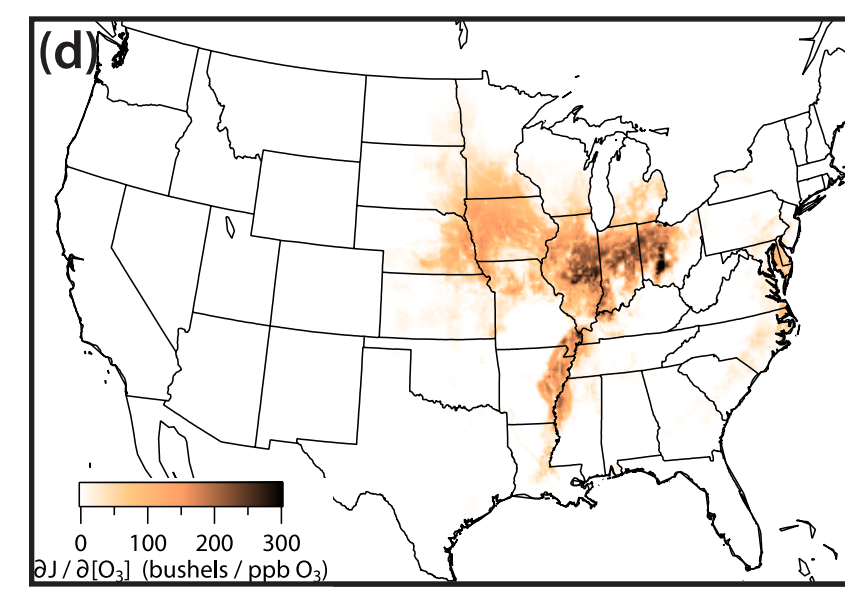
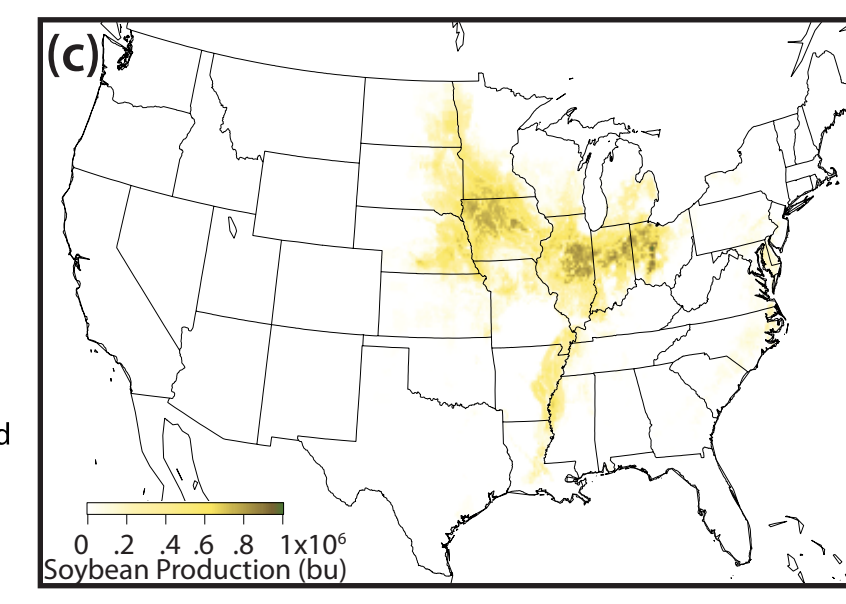
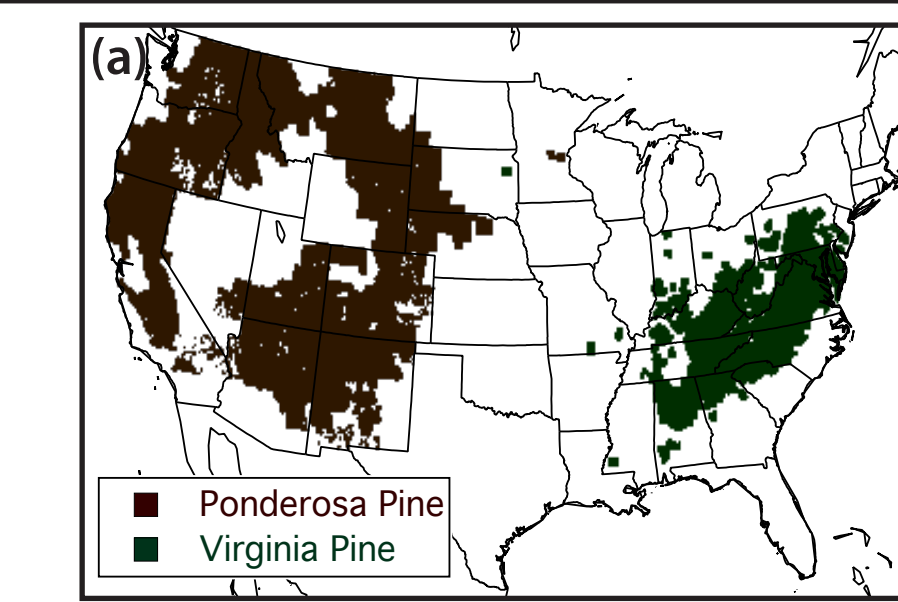
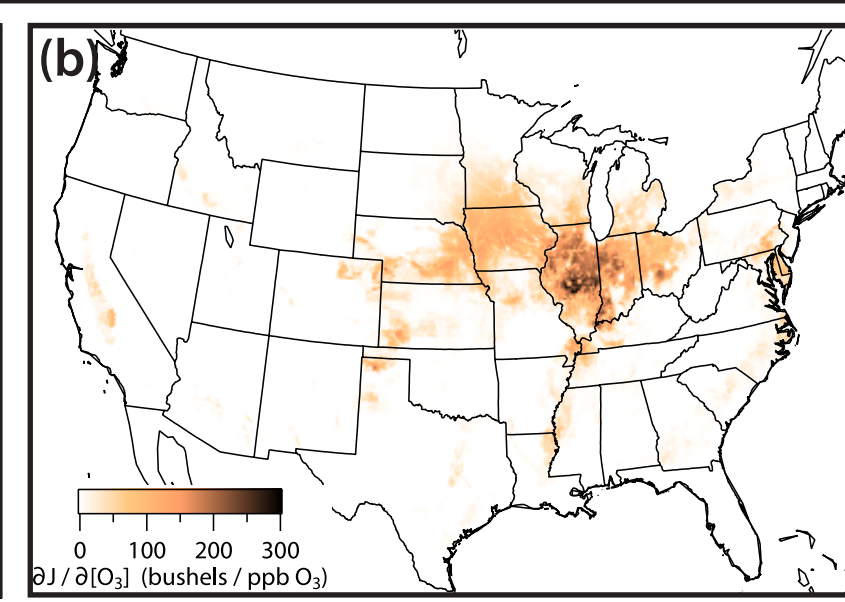
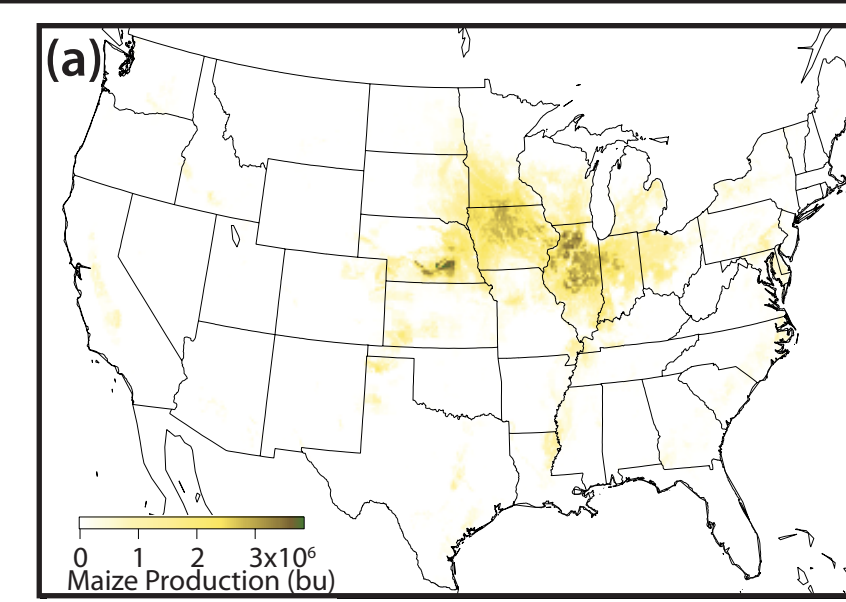


Figure 13. 2007 production of maize (a) and soybean (c) in bushels. The distribution and amount were reconstructed from NASS production statistics and BELD land use data. The effect of incremental ozone increase on crop production is based on the 2007 ozone concentrations.

The seasonal yield loss is distributed across grid cells in accordance with the contribution the ozone in each cell and hour made to the total W126. The forcing is always zero at night to reflect the closing of the plant stomata. Additionally, the sensitivity of productivity to the W126 metric for maize (Fig. 13b) and soybeans (Fig. 13d) are allocated according to the actual yield in the grid cell (Fig. 13a,c). Tree species are located even more disparately (Fig. 14a); the wider range of responses to W126 is evident in the magnitude of response for Douglas Fir and Virginia Pine. The differences in the spatial patterns and magnitude between the different tree species and crops arise from unique distributions and yields (for crops) as well as W126 dose-responses.

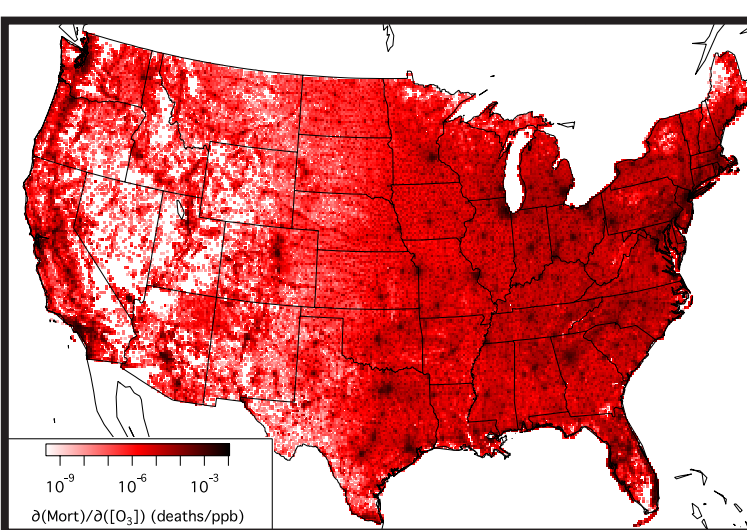
Figure 14. The distribution of tree species was reconstructed from Forest Inventory and Analysis data from the US Department of Agriculture (a). Two sample species, Ponderosa Pine and Virginia Pine, are shown but eight different trees have associated adjoint forcing functions prepared. The effect of incremental ozone increase on timber production (b) is based on the 2007 ozone concentrations. Ponderosa Pine and Virginia Pine were two of the most affected tree species in 2007.

## V. Current Message & Next Steps

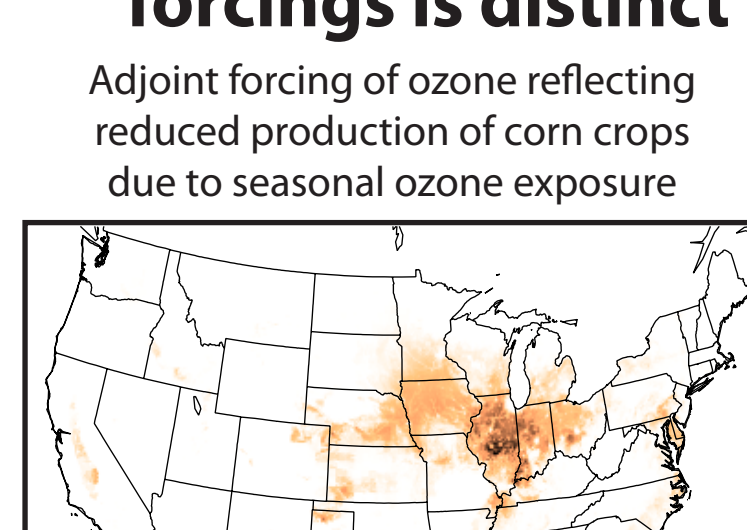
### Modeling developments

Incremental changes in ozone concentration in the summer months can now be propagated to effects on mortality (Jerrett et al. (2009)) or crop and timber yield losses as a function of the W126 metric in Python-based CMAQ adjoint preprocessor. Additionally, spatially-distributed primary crop yields and biomass presence have been constructed for 2007.

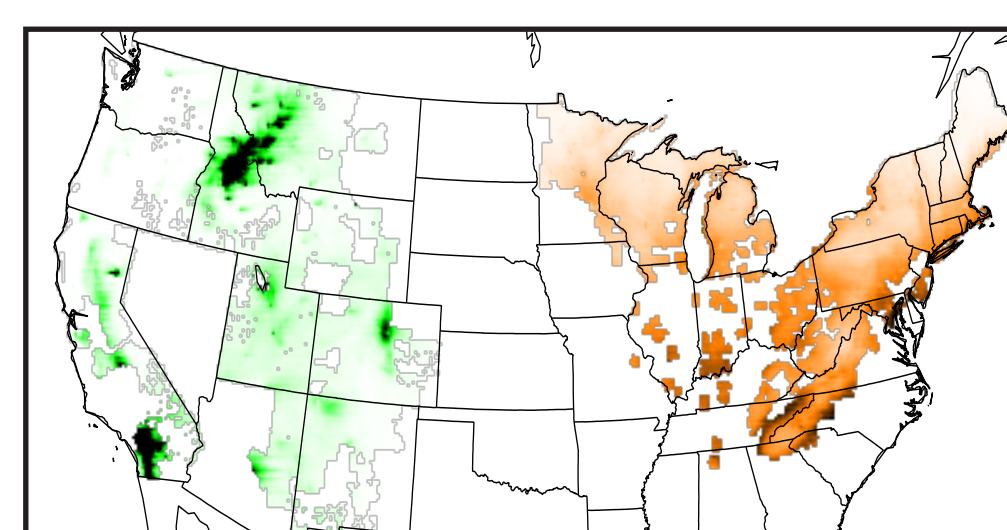
### Spatial patterning of health & ecosystem forcings is distinct



Adjoint forcing of ozone reflecting mortality from respiratory causes due to long-term ozone exposure



Adjoint forcing of ozone reflecting reduced production of corn crops due to seasonal ozone exposure



Adjoint forcing of ozone reflecting reduced production of timber due to seasonal ozone exposure

### Relative Importance to Tree Type

The most significantly affected tree types in 2007 were *Ponderosa Pine*, *Virginia Pine*, and *Red Alder*. The trees most resistant to ozone impacts or located in areas with lower ozone concentrations are *Douglas Fir*, *Sugar Maple*, and *Tulip Tree*. Next, the system will incorporate biomass distribution as well as presence.

Finally, we will **apply these adjoint forcings within the CMAQ adjoint framework** to observe any distinction between emissions influences on each regulatory endpoint.

## VI. References & Acknowledgements

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