Importance of model complexity on modeling ambient air quality and the resulting health impacts

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Science Question

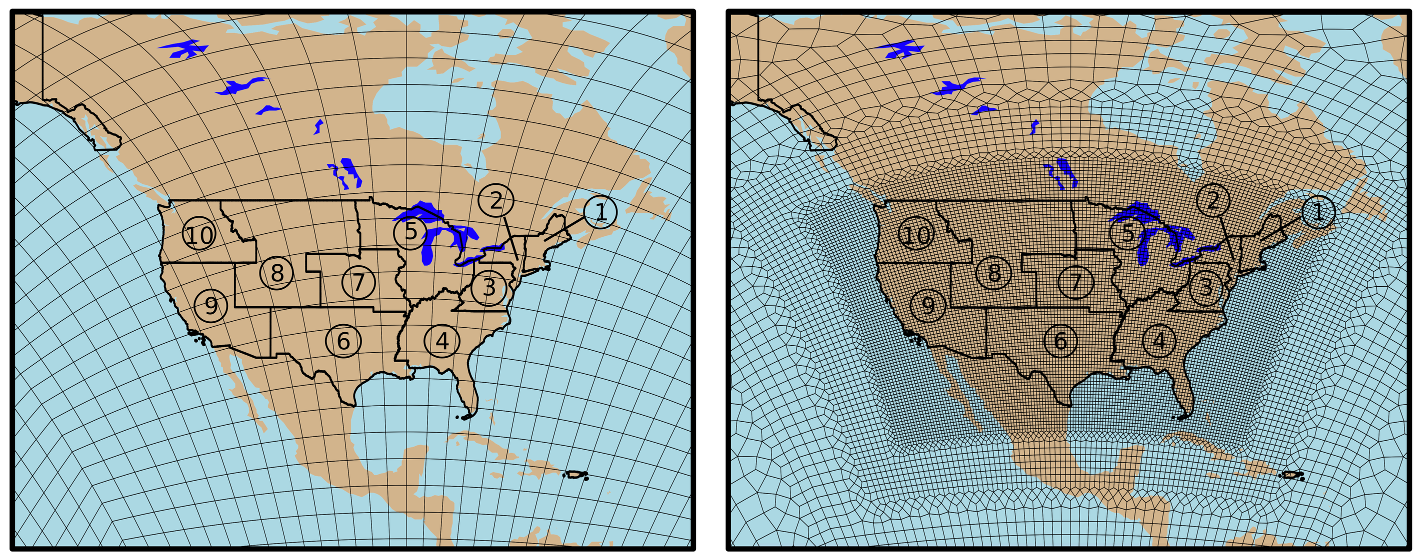
Models are often used to predict ambient air quality and the burden of disease associated with exposure to trace pollutants in the atmosphere. As models have become increasingly complex through more complex chemical mechanisms and higher horizontal resolutions, little work done in quantifying the impact on the burden of disease associated with these changes and uncertainties that can be tied to model complexity.

Model Framework

MUSICA.v0 allows for modeling of the formation and fate of trace pollutants at different resolutions and using various chemical mechanisms

Horizontal Scale:
Global 1° degree cubed-sphere
Global 1° with 1/8° degree over CONUS

Chemical Complexity:
MOZART TS1 – 151 species
MOZART TS2 – 237 species (improved isoprene and terpene chemistry, Schwantes et al., 2020)



Lacey et al., *in prep*

Experimental Setup

In order to look at the impacts of model horizontal resolution, we used the spectral element dynamical core that allows for model calculations on an unstructured model grid. Using this we created a grid over CONUS that scales down to one eighth degree while including the full globe at a coarser one degree all within the same simulation. The results from this run were compared to a standard one degree grid throughout the globe. Shown on the maps above are also the outlines of the EPA regions that we used from analysis of the results.

Run ID	Horizontal Resolution	Chemical Mechanism	Emissions Resolution
1DEG - TS1	SE ne30np4 1° cubed-sphere	MOZART TS1 151 Species	1° cubed-sphere
1DEG - TS2	SE ne30np4 1° degree cubed-sphere	MOZART TS2 237 Species	1° cubed-sphere
RR - TS1	CONUS ne0np4-30x8 1° global to ⅛° over CONUS	MOZART TS1 151 Species	⅛° over CONUS
RR - TS2	CONUS ne0np4-30x8 1° global to ⅛° over CONUS	MOZART TS2 237 Species	⅛° over CONUS

To explore chemical complexity we have used two different chemical mechanisms. The first is that standard MOZART TS1 mechanism used in CAM-chem that includes over 150 species and their corresponding reactions related to the formation of both gaseous and aerosol trace pollutants and include simplified VBS based SOA formation. The second mechanism include over 80 additional species and focuses on improved estimation of the oxidation products from isoprene and terpene chemistry; something that has been shown to have a significant impact on summertime ozone estimation. The version of MOZART TS2 used here also includes a high-NOx pathway for SOA formation, therefore further impacting estimates of PM2.5.

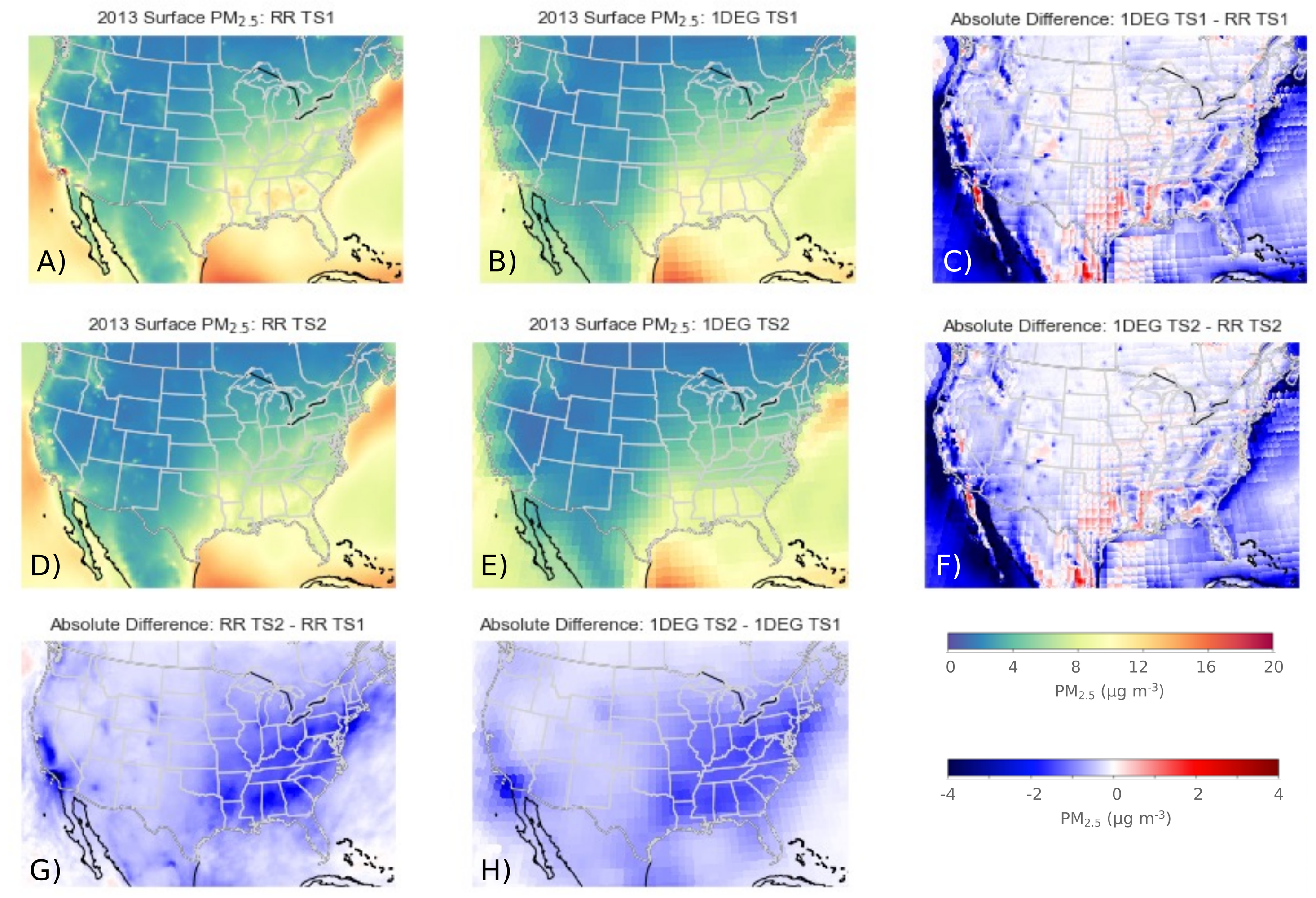
References:

Pfister, G. G., Eastham, S. D., Arellano, A. F., Aumont, B., et al.: A MUlti-Scale Infrastructure for Chemistry and Aerosols - MUSICA, Bull. Amer. Meteor. Soc., 1–50, https://doi.org/10.1175/BAMS-D-19-0331.1, 2020.

Schwantes, R. H., Emmons, L. K., Orlando, J. J., Barth, M. C., et al.: Comprehensive isoprene and terpene gas-phase chemistry improves simulated surface ozone in the southeastern US, 20, 3739–3776, https://doi.org/10.5194/acp-20-3739-2020, 2020.

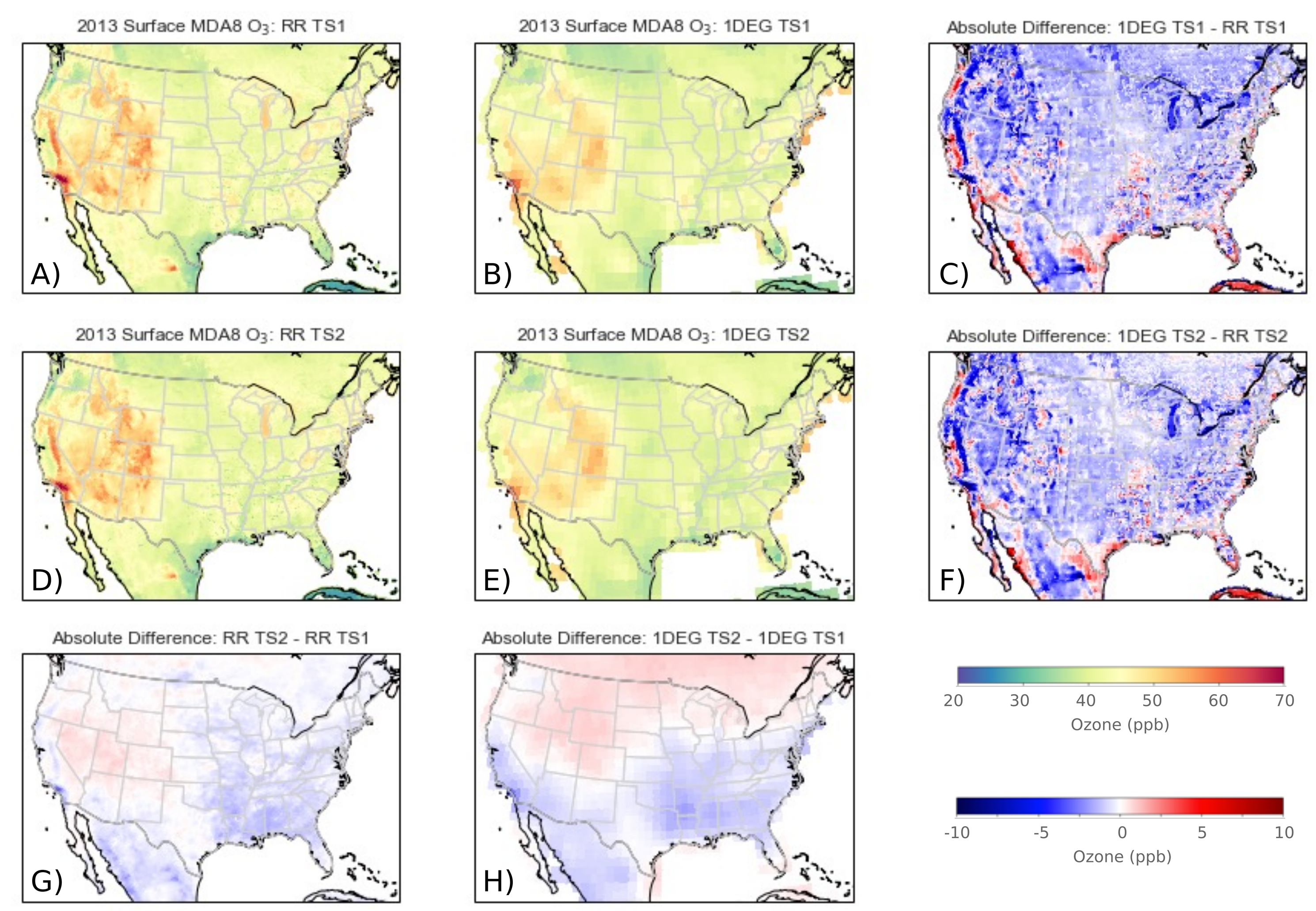
Annual $PM_{2.5}$ Concentration Shifts

The plots show the annual $PM_{2.5}$ concentrations for each simulation with the difference plots on the right showing changes due to resolution and the bottom plots showing differences from increased chemical complexity. Throughout the west, areas of bright blue are due to wildfire activity dispersing localized emissions over a larger area and concentrations near the coasts are due to better resolved coastlines in addition to higher wind speeds calculated in the regionally refined case. The addition of TS2 chemistry reduces SOA formation through improvements in speciation and NOx influenced pathways leading to changes in regions dominated by biogenic emissions. Overall changes in chemical complexity (G & H) and those to resolution (C & F) have similar order of magnitude impacts on $PM_{2.5}$ concentrations although vary spatially.

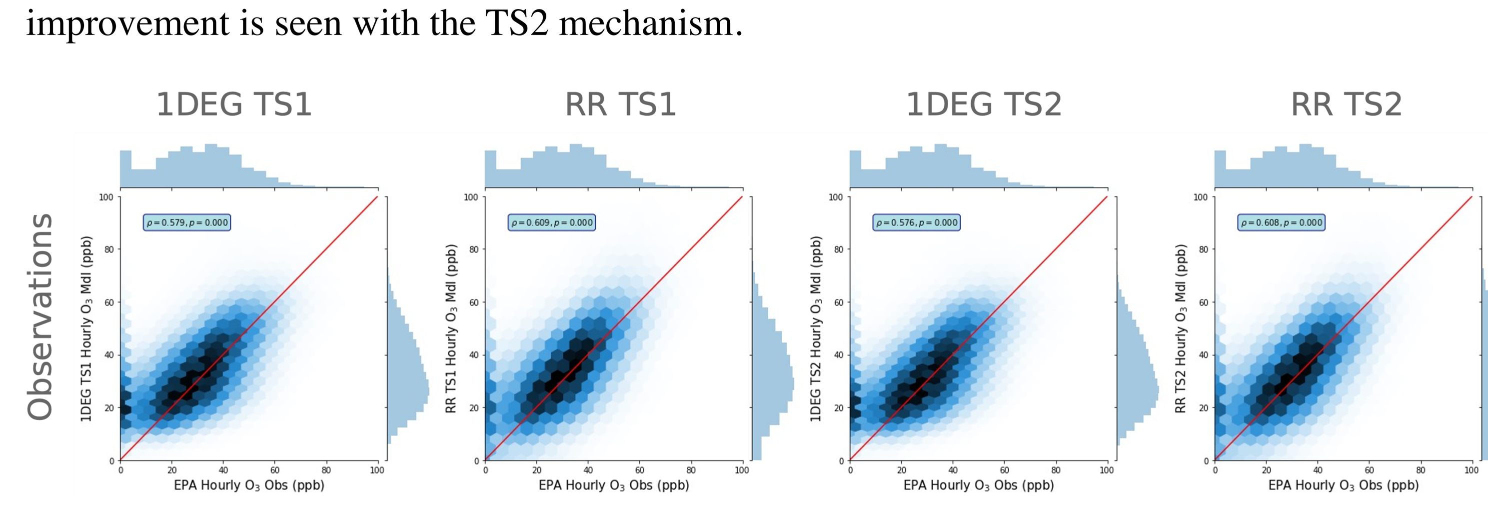


Annual Ozone Concentration Shifts

For changes in horizontal resolution, two impacts present the largest impacts on annual concentrations of maximum daily 8-hour (MDA8) ozone; complex topography affecting transport and localized emissions near population centers. Unlike $PM_{2.5}$ concentrations, shifts in ***annual*** ozone concentrations due horizontal resolution are larger than those due to chemical complexity (note: while not as large of a contribution to annual concentrations, significant improvements in ***summertime*** ozone are realized with additional chemical complexity).



Hourly concentrations are also compared to all available hourly observations from the EPA AQS network. Improvement is shown for the regionally-refined model, although no significant improvement is seen with the TS2 mechanism.



Generalized Heath Impact Functions

$$\Delta Mort = y_{0,s,y}(1 - exp^{-\beta_y \Delta X_{i,y}})Pop_i$$

Baseline Incidence Rates
Source:
CDC WONDER
(hospital records)

Resolution:
Annual (y)
State-level (s)

Hazard Ratio
Source:
Burnett et al., 2018
Turner et al., 2016
Malley et al., 2018
(cohort studies)
$1.12 = exp^{-\beta 10ppb}$

Resolution:
Annual Exposures (y)

$PM_{2.5}$ Concentration
Source:
MUSICAv0

Resolution:
Annual Concentrations (y)
Grid cell (i)

Population
Source:
ORNL Database
(census data fusion product)

Resolution:
Aggregated to grid cell (i)

Health Impact Results

Using the modeled concentrations and health impact functions we have calculated the annual attributable deaths for each EPA region for both $PM_{2.5}$ and ozone. The deaths for each run is shown on the left and the differences for horizontal resolution (purple) and chemical complexity (orange) are shown on the right.

Conclusions and Future Work

Initial experiments show that both horizontal scale and chemical complexity are of equal importance for estimating non-linear species such as ozone and PM2.5, especially when considering localized or regional impacts

Attributable Deaths		
Run	**PM2.5**	**Ozone**
1DEG TS1	71719	30052
RR TS1	90639	34416
RR TS2	72994	34259

Next set of simulations will include a number of changes such as diurnal emissions scaling, inclusion of nitrate aerosols, and updated emissions

Work with epidemiologists to better include errors due to assumptions of health-relevant functions and data (i.e. what is the error due to shifts in HR)