Using SEAC⁴RS observations to understand impact of grid resolution on chemical transport modeling

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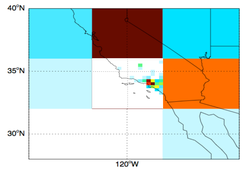
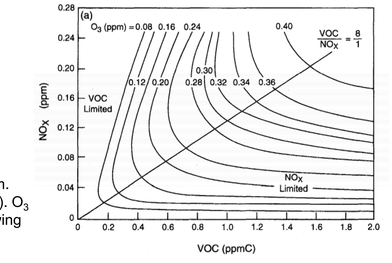
MOTIVATION

GEOS-Chem recently introduced the capability to run at 0.25ºx0.3125º resolution over several nested domains. Given the computational cost of running a high resolution model, it is important to quantify the benefits of increased resolution and identify applications where a high resolution model is necessary and applications where running at coarse resolution is sufficient. SEAC⁴RS offers an opportunity to constrain resolution related uncertainties in the GEOS-Chem model and quantify the added value of a high resolution chemical transport model.

How does grid resolution affect a model?

Atmospheric processes span a wide range of scales, many of which cannot be resolved on typical grid sizes used in global atmospheric chemistry models. Sub-grid interactions between species can induce biases in the model when the model only has access to the grid volume mean values. Previous work found that a higher resolution model produces less ozone in polluted boundary layers and exports more ozone precursors[1], and that peak ozone can be underestimated in coarse resolution models[2]. In addition to non-linear chemistry, grid resolution can also impact numerical diffusion as well as emissions and other inputs.





Left: Spatial scale of NO_X emissions in GEOS-Chem. **Right**: Figure 1 from Finlayson-Pitts and Pitts (1993). O_3 isopleths for different levels of NO_x and VOCs, showing non-linearity of O_3 response to emissions.

Overall model performance

Differences in model performance for the low and high resolution simulations are generally small when measured in terms of Pearson's correlation coefficient and root mean square error (RMSE).

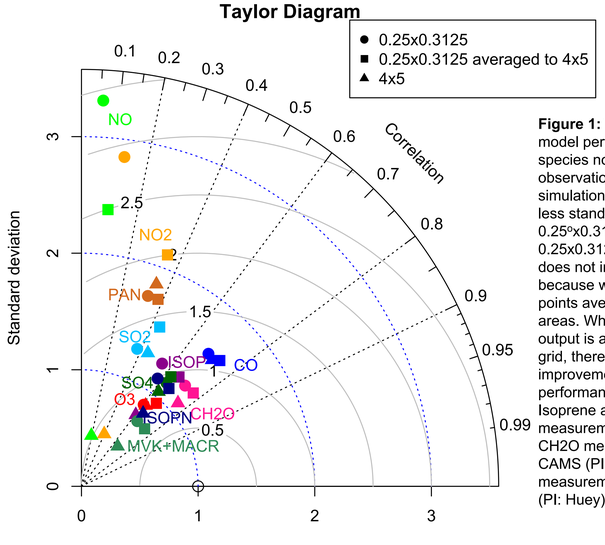


Figure 1: Taylor Diagram of model performance for various species normalized to observations. The 4ºx5º simulation generally captures less standard deviation than the 0.25ºx0.3125º simulations. The 0.25x0.3125 simulation often does not improve correlations because we are comparing points averaged over smaller areas. When the 0.25ºx0.3125º output is averaged to the 4ºx5º grid, there are small improvements in model performance for some species. Isoprene and MVK+MACR measurements from Wisthaler. CH2O measurements from CAMS (PI: Fried), PAN measurements from GTCIMS (PI: Huey).

Methodology for comparisons

Data type	DC8 60s merges	GEOS-Chem global	GEOS-Chem nested
Grid	None	4ºx5º 60 min time-step	0.25ºx0.3125º 10 min time-step

GEOS-Chem was run at both global 4x5 resolution and N. America nested 0.25x0.3125 resolution for the SEAC4RS campaign period with data saved out at 60s timesteps along the flight track. Flight data is averaged to the GEOS-Chem grids for computing correlations. In all figures, 'avg' denotes GEOS-Chem output at 0.25x0.3125 resolution averaged to the 4x5 grid.

Background vs. urban

Differences in model performance are larger when looking at urban plumes separately from the background. Ozone concentrations in regions of high NOx emissions will be more impacted by resolution because a coarse resolution model is unable to resolve intense point sources. Commonly used model evaluation metrics suggest that increased resolution improves model performance for a non-linear species like ozone, but not for CO which has simpler chemistry..

Metric	Resolution	O3		CO		NOx		SO2		SO4	
		Urban	Bkgd	Urban	Bkgd	Urban	Bkgd	Urban	Bkgd	Urban	Bkgd
NMB (%)	4x5	22.7	17.6	-25.7	-8.14	-62.0	30.7	-29.7	67.3	-20.9	-25.3
	0.25x0.3125	7.72	17.1	-37.4	-6.01	91.7	32.2	-42.4	48.4	-25.4	-13.1
	Avg	17.9	21.0	-17.7	-3.17	32.4	32.8	-23.9	60.6	-18.1	-13.1
NME (%)	4x5	38.2	25.4	35.2	24.9	77.0	67.0	77.5	125	38.9	59.2
	0.25x0.3125	32.4	26.9	46.7	26.5	213	76.4	76.6	119	49.1	56.6
	Avg	35.4	27.2	36.9	24.9	115	66.8	72.4	123	39.2	56.2
RMSE (ppb, ppt, ug/m³)	4x5	25.4	18.4	120	32.8	2.38	0.192	711	431	1.10	1.32
	0.25x0.325	29.3	20.2	303	36.1	8.45	0.291	1040	482	1.28	1.38
	Avg	24.6	19.2	121	33.8	4.20	0.194	651	481	1.03	1.36

Table 1: NMB, NME, and RMSE for various species compared to observations. Urban refers to data points where NO_2 > 4 ppbv or NO_2/NO_y > 0.4. Background (Bkgd) refers to data after filtering for fire and urban plumes. O_3 and NOx measurements from ESRL (PI: Ryerson), SO_2 from GTCIMS (PI: Huey) and SO_4 from SAGA (PI: Dibbs).

Ability to capture tails of distribution

For certain modeling applications, it is important to capture not only the mean, but also the tails of the distribution of the actual values (for example, modeling ozone exceedances). Even if a high resolution model and a coarse resolution model have similar ability to capture the center of a distribution, the high resolution will be better able to capture the tail.

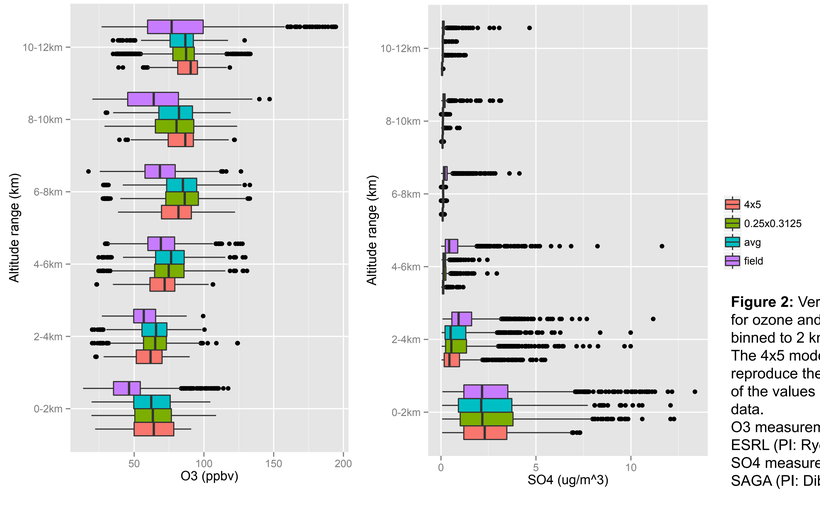


Figure 2: Vertical profile for ozone and SO_4 binned to 2 km ranges. The 4x5 model does not reproduce the high end of the values seen in the data.
O3 measurements from ESRL (PI: Ryerson) and SO4 measurements from SAGA (PI: Dibbs).

Correlations between species

Correlations between different chemical species can be used to constrain sources and processes contributing to the burden of a species. Even if two models produce similar concentrations of a species, it may be the result of different processes.

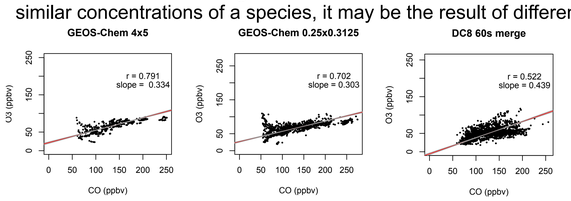


Figure 3: Ozone-CO correlations for data points in the planetary boundary layer. CO observations from DACOM (PI: Diskin).

Detailed features in high resolution model

Although when compared on a point by point basis, a higher resolution model doesn't always perform better than a coarse resolution model, it undeniably produces more smaller scale features that cannot be resolved in a coarse resolution model. If a small-scale feature in the model is displaced spatially or temporally from its actual location, the model will not compare favorably to observations using traditional model evaluation metrics. Future will work use LIDAR data to evaluate the model's ability to reproduce small scale features.

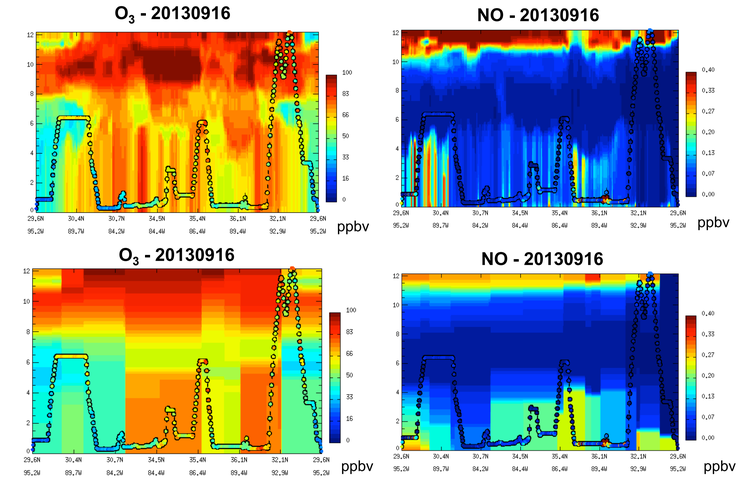


Figure 4: Model curtain along flight track overplotted with in-situ observations. Ozone and NO observations from ESRL (PI: Ryerson).

As computational power increases to allow higher resolution atmospheric models, it is important to quantify the benefits of increasing model resolution. **The necessary resolution is highly dependent on the application of the model**: modeling the continental background appears to not require as high resolution as urban areas. **Commonly used model evaluation metrics are unable to distinguish between displacement and amplitude errors** and therefore may undervalue high resolution models. Future work will provide more quantitative evaluations of model performance at different grid resolutions.

References

Finlayson-Pitts, B. J., and J. N. Pitts Jr. "Atmospheric chemistry of tropospheric ozone formation: scientific and regulatory implications." *Air & Waste* 43.8 (1993): 1091-1100.
[1]Wild, Oliver, and Michael J. Prather. "Global tropospheric ozone modeling: Quantifying errors due to grid resolution." *Journal of Geophysical Research: Atmospheres (1984–2012)* 111.D11 (2006).
[2]Kumar, Naresh, and Armistead G. Russell. "Multiscale air quality modeling of the northeastern United States." *Atmospheric Environment* 30.7 (1996): 1099-1116.