Scale Dependency of Model Estimates for Nitrogen Dioxide Concentrations in the Western United States

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Motivation

Regional air quality modeling systems such as the Community Multi-scale Air Quality (CMAQ) model driven by the Weather Research and Forecasting (WRF) meteorological model are often used to estimate ambient pollutant concentrations at high temporal and spatial resolutions. Nitrogen dioxide (NO_2) in the atmosphere is an air pollutant considered harmful to public health and the environment and is regulated by the U.S. Environmental Protection Agency under the Clean Air Act. Accurate prediction of NO_2 and other pollutant concentrations is critical for the development and implementation of air quality control rules and regulations.

The WRF-CMAQ simulations for 1997-1998 using a 12-km x 12-km grid for the western U.S. consistently underestimate NO_2 concentrations (Fig. 1). The model performs poorly in urban and suburban areas, with fractional biases averaging ~45% on a monthly basis and around 25% in rural areas. Systematic and in-depth analyses are needed to better understand the reasons for model biases. Questions of interest include which time scales dominate the variances in NO_2 concentrations and how well does the model predict these variances.

Model Errors for Hourly NO_2 concentration

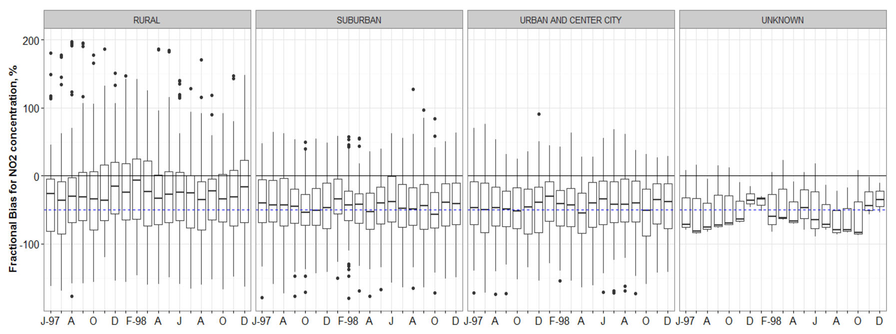

Fig. 1 Monthly Fractional Biases (FB) for hourly NO_2 concentration grouped by site characteristics over the two year analysis period.

Objectives

- Examine distribution of hourly NO_2 concentration time series.
- Evaluate model performance of NO_2 concentrations at distinct temporal scales.

Data and Methods

- Hourly NO_2 concentrations measured at 249 sites were obtained from the EPA's Air Quality Service (AQS).
- Hourly NO_2 concentration outputs from the WRF-CMAQ modeling framework were extracted from grid cells covering the sites for the time period of June 1997-December 1998.
- The log-transformed NO_2 time series were decomposed into four temporal scales using the Kolmorgorov-Zurbenko filtering technique[2]:

intra-day (<11 hours): $ID(t) = \ln[O_3(t)] - KZ_{3,3}\{\ln[O_3(t)]\}$

diurnal (11-36 hours): $DU(t) = KZ_{3,3}\{\ln[O_3(t)]\} - KZ_{13,5}\{\ln[O_3(t)]\}$

synoptic (2.5- 21 days): $SY(t) = KZ_{13,5}\{\ln[O_3(t)]\} - KZ_{103,5}\{\ln[O_3(t)]\}$

long term (> 21 days): $BL(t) = KZ_{103,5}\{\ln[O_3(t)]\}$

- Correlation and variance analysis were carried out on observed and modeled NO_2 concentration time series and by site characteristics (rural, urban, suburban) and dominant emission source types (agricultural, residential, and mobile) for each temporal scale.

Observed and Predicted Component Variances

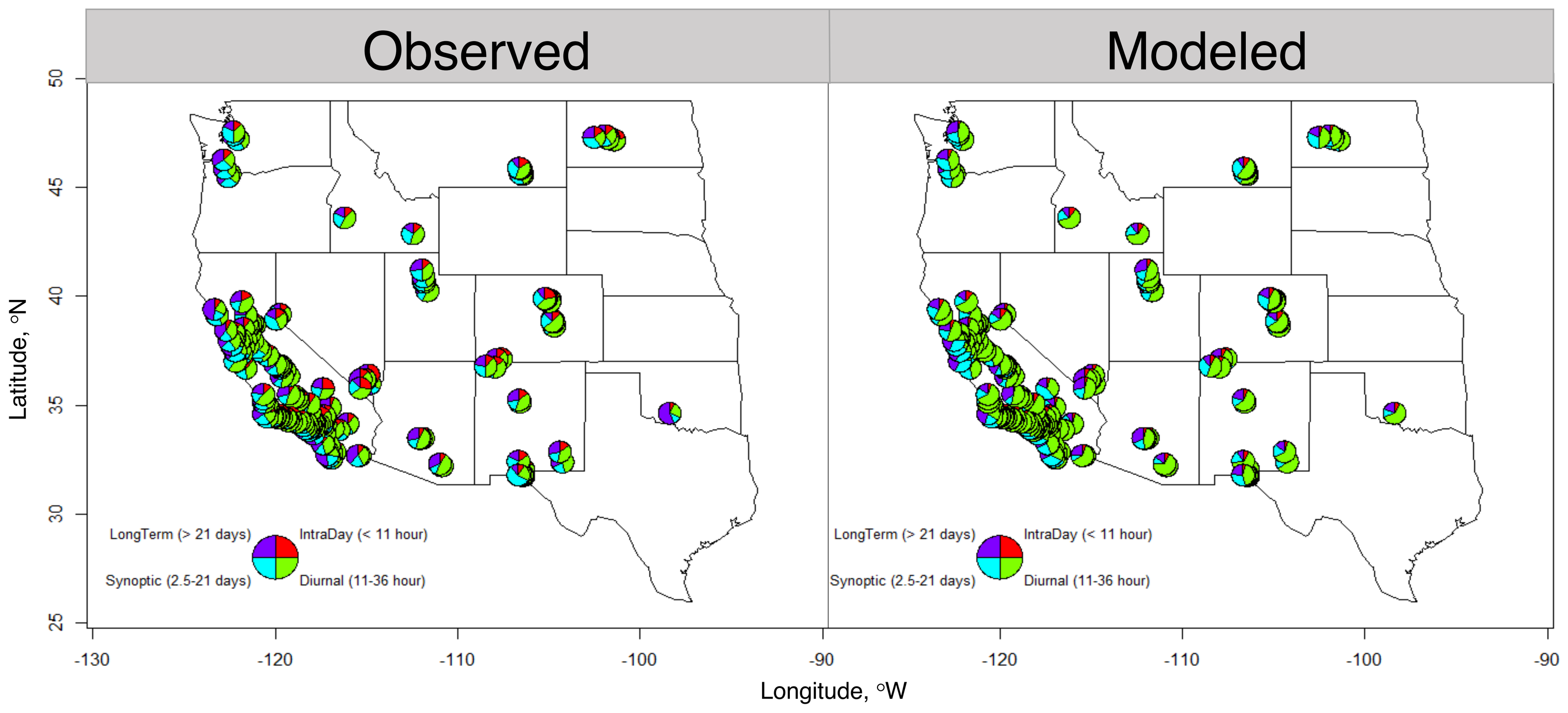

Fig. 2 Relative contributions of the four temporal components embedded in the observed (left) and modeled (right) NO_2 concentration time series. The model overestimates contribution from the diurnal timescale and underestimates that from the intra-day timescale.

Site Location Setting	# of sites	Mean NO_2, ppbV		Average variance for ln (NO_2)		Intra-day		Diurnal		Synoptic		Long-term		Sum of partial variances	
		Obs	Mod	Obs	Mod	Obs	Mod	Obs	Mod	Obs	Mod	Obs	Mod	Obs	Mod
Rural	63	6.9	5.1	0.54	1.01	13%	4%	27%	37%	17%	17%	16%	15%	73%	73%
Suburban	69	18.5	13.6	0.51	0.81	8%	4%	28%	35%	17%	18%	22%	17%	75%	73%
Urban and Center City	51	20.7	14.9	0.47	0.77	8%	4%	27%	36%	17%	16%	23%	17%	77%	74%
Unknown	3	12.4	8.1	0.58	0.92	7%	4%	26%	33%	15%	18%	28%	19%	75%	73%

Table 1. Total and partial variances of the four different temporal components by site characteristic. Blue and orange indicate that the model underestimates and overestimates, respectively, by at least 25%.

Correlations Between Observed and Predicted Components

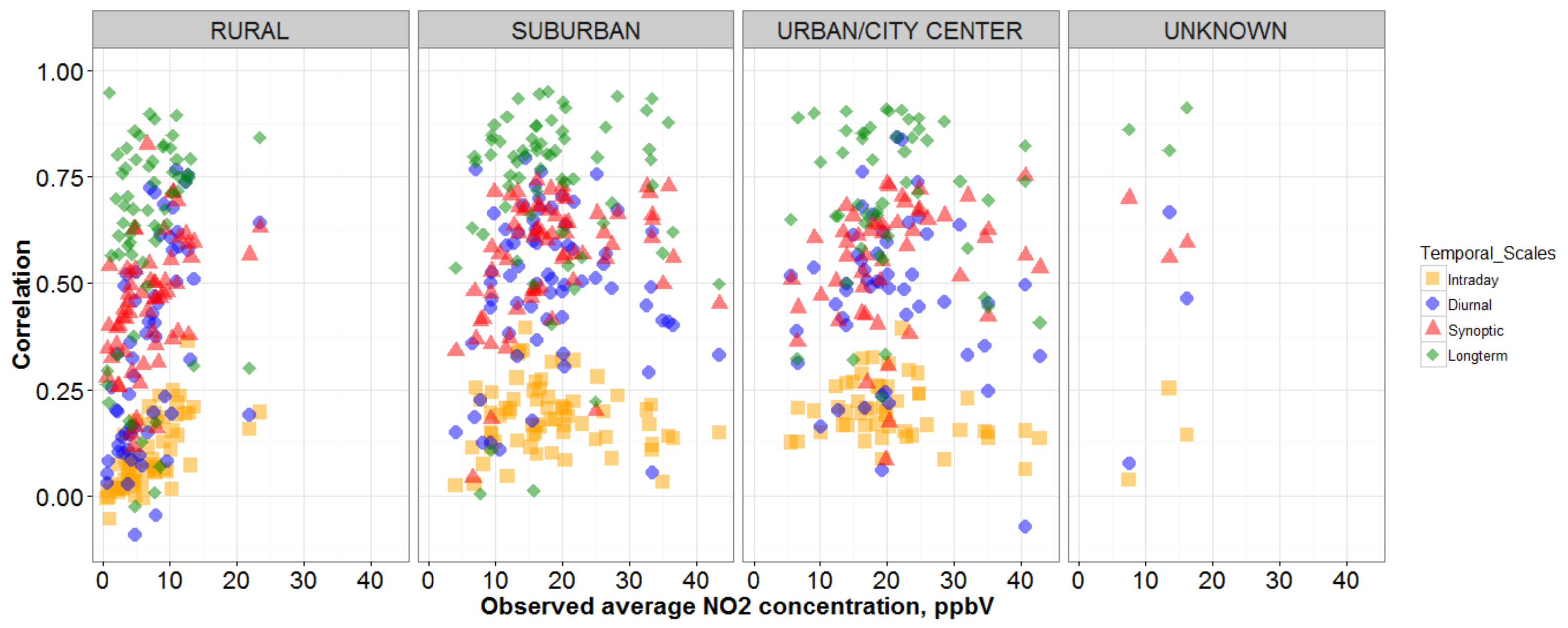

Fig. 3 Pearson's correlations between decomposed modeled and observed NO_2 time series for each type of site. The *x*-axis shows observed mean NO_2 concentration at each site.

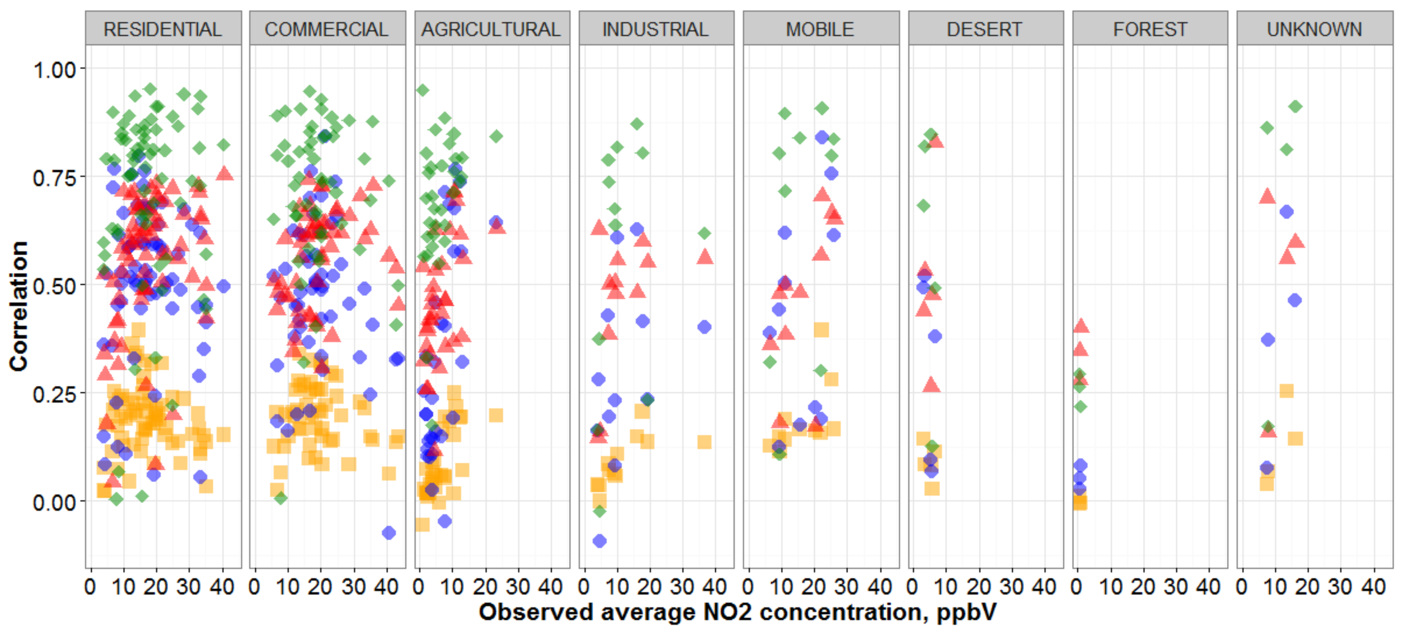

Fig. 4 Pearson's correlations between decomposed modeled and observed NO_2 time series at each AQS sites. The sites are grouped by the dominant emission sources. The *x*-axis shows observed mean NO_2 concentration at each site.

Discussions

- Kolmorgorov-Zurbenko filtering was applied to log-transformed NO_2 time series for all sites. Site-by-site analysis on NO_2 time series indicates that log-normal or gamma distribution provides the best fit. Of the 104 sites for which a gamma distribution is a better fit than a log normal distribution, gamma distribution is only marginally better.
- Averaged over all sites and the study period, for the observed NO_2 time series, the diurnal, long-term and synoptic components contributed 34%, 32%, and 22%, respectively, to the total variance (Fig. 2).
- While modeled NO_2 time series contains similar relative contributions, the model overestimates contribution from the diurnal component and underestimates contribution from the long-term component (Fig. 2, Table 1).
- The intra-day component contributed 11% in the observed NO_2 time series, but only 5% in the modeled time series (Table 1).
- There is a trend associated with higher correlations and length of temporal scale; however, correlations between modeled and observed diurnal and long-term components display large variability (Figs. 3 & 4).
- No systematic differences are seen in correlation patterns associated with site characteristics that were examined in this study (Figs. 3 & 4).

Future Work

- Segregate hourly NO_2 concentrations into three temporal scales in order to maximize optimal condition of the Kolmorgorov-Zurbenko filtering.
- Conduct similar analysis on modeled NO_x emissions, concentrations of other species involved in NO_x-ozone chemistry, and meteorological variables to identify reasons for model-observation discrepancies.
- Explore other scale separation techniques such as the Lomb–Scargle periodogram.

References and Acknowledgments

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