APPLICATION OF WAVELET FILTERS IN AN EVALUATION OF PHOTOCHEMICAL MODEL PERFORMANCE

P. Steven Porter[1], Christian Hogrefe[2], Edith Gégo[3], Kristen Foley[4], James Godowitch[4], and S.Trivikrama Rao[4]

[1]University of Idaho, Idaho Falls, ID, U.S.A., [2]ASRC, University at Albany, Albany, NY, U.S.A., [3]GEGO and Associates, [4]Atmospheric Modeling & Analysis Division, U.S. Environmental Protection Agency

1. INTRODUCTION

Air quality model evaluation can be enhanced with time-scale specific comparisons of outputs and observations. For example, high-frequency (hours to one day) time scale information in observed ozone is not well captured by deterministic models and its incorporation into model performance metrics lead one to devote resources to stochastic variations in model outputs. In this analysis, observations are compared with model outputs at seasonal, weekly, diurnal and intra-day time scales. Filters provide frequency specific information that can be used to compare the strength (amplitude) and timing (phase) of observations and model estimates.

2. METHODS AND TIME SERIES

2.1 Modeling system

Model outputs were produced by MM5-v3.7.2, CMAQ-v4.5.1, CB4 and aero3 set to simulate the time period 1988–2005 (Hogrefe et al, 2009). The domain was the northeastern U.S. at a grid of 12 km x 12 km. Emissions included NEI 1990, 1996-2001, OTC2002, and OTC2009, processed by SMOKE .

2.2 Observations

Observations (ozone concentrations and meteorological variables) used for time series examples were recorded by the *Clean Air Status and Trends Network* (CASTNET, www.epa.gov/castnet/data/metdata/) operated by the Environmental Protection Agency's Clean Air Markets Division. CASTNET sites are located in mostly rural and remote areas such as national parks and monuments. Illustration of weekly variation in ozone was demonstrated with ozone data from the EPA's air quality system (www.epa.gov/ttn/airs/airsaqs/detaildata/downloadaqsdata.htm).

CASTNET sites and CMAQ grid cells at Abington, CT (ABT147) and Shenandoah National Park, VA (SHN418) were chosen for purposes of illustration. ABT is downwind of the New York City urban area. SHN is a high altitude site (elev. 1,073 m).

2.3. Low pass filter (KZ)

A low-pass filter (iterative moving average where high frequencies are damped and low frequencies are unaltered) was used to define the trend (KZ(k=3 iterations, q=182 days) and intra-day (original - KZ(k=3 iterations, q=1 hour)) time scales (Zurbenko, 1986; Rao and Zurbenko, 1994). An advantage of the KZ over other linear filters is its ease of application when some observations are missing: missing values are ignored and a mean is computed from whatever values are present. Endpoints of time series (as well as the edges of gaps) are not properly filtered and are therefore clipped when presented.

2.4. *Wavelet filter*

The KZFT(q,k,w) wavelet is a Fourier transform (FT) version of the KZ (Zurbenko and Porter, 1998). The KZFT is given by:

$$Y_t = \frac{1}{2q+1} \sum_{k=-q}^{+q} \exp(-\ i\ 2\ \pi\ \omega\ k) \cdot X_{t+k} \tag{1}$$

where q is the half-window size and k is the number of iterations, T is a frequency of interest, and 'i' is $(-1)^{1/2}$. The real part of the filtered time series, $Y(Y_t)$, is a bandpass component centered at frequency T, and $|(Y_t)|$ is the instantaneous amplitude of Y(t).

Cross-correlations do not adequately describe relationships among different periodic processes. Any two time series with seasonal (or diurnal) variation will tend to be highly correlated when adjusted for phase difference. As such, it's better to compare amplitudes and phases. Consider the following conceptual model for seasonal variation:

$$Q_{se} = A_t \cdot \cos\left(\frac{2\pi t}{p} + ph_t\right) \tag{2}$$

where Q_{se} is seasonal variation in a process Q at time t, A_t is the amplitude of seasonal variation at time t, p is the period (one year) and ph_t is the phase at time t. Seasonal phase is calculated from (Bloomfield, 2000):

$$ph_t = \Im\left[\ \ln \frac{Y_t \cdot \exp(-i \cdot 2 \cdot \pi \cdot t \cdot \omega)}{\mathrm{abs}(Y_t \cdot \exp(-i \cdot 2 \cdot \pi \cdot t \cdot \omega))}\right] \tag{3}$$

and can be thought of as the day of the year that a process reaches a maximum. An estimate of A_t is the modulus of the wavelet filtered time series. Phase (ph_t) and amplitude (A_t) of seasonal ozone are typically low frequency processes.

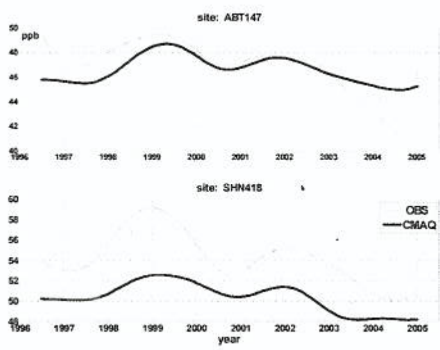

Figure 1. Observed and modeled trend (low-frequency variation) at ABT and SHN

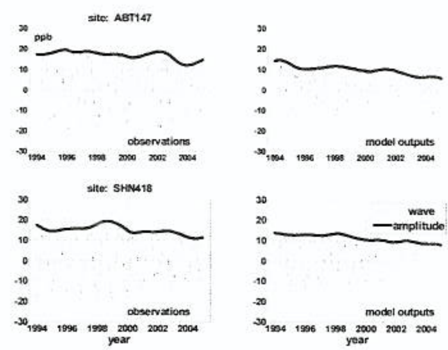

Figure 2. Observed and modeled seasonal variation at ABT and SHN

3. RESULTS AND DISCUSSION

3.1. Observed and modeled ozone by time scale

Low-frequency ozone variation (trend) was defined with a low-pass filter (Figure 1). The trend is captured by CMAQ (R = 0.79 and 0.89 at ABT147 and SHN418, respectively).

Observed and CMAQ seasonal wavelets and their amplitude for ABT and SHN are shown in Figure 2. Correlations between observed and CMAQ seasonal variation (0.97 and 0.99 at ABT and SHN, respectively), for the most part measure phase differences.

Among the meaningful measures of agreement between observations and model outputs are the correlation between seasonal amplitudes (0.71 and 0.76 at ABT147 and

SHN418, respectively) and the phase difference (Figure 3). CMAQ is out of phase with observations, sometimes by more than 10 days. The CMAQ phase has trended downward since 1999 at both sites (seasonal maximum coming earlier).

Ozone seasonal amplitude is modulated in part by meteorology (Figure 4). The dotted lines in Figure 4 are linear combinations of meteorological variables that include temperature, solar radiation, relative humidity and wind speed. The most significant covariates are wind speed and solar radiation at ABT and SHN, respectively.

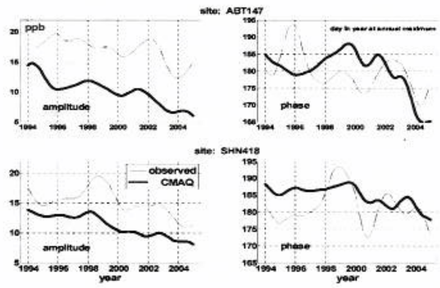

Figure 3. Observed and modeled seasonal amplitude and phase at ABT and SHN

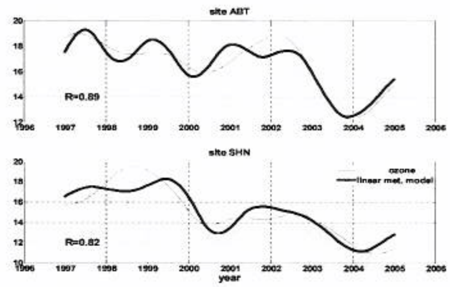

Figure 4. Seasonal amplitude and linear meteorological model for ABT and SHN

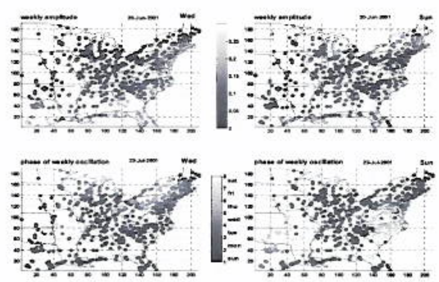

Figure 5. ABT weekly amplitude (log of ppb) a) 20 June and b) 22 July and weekly phase c) 20 June d) 22 July

Weekly amplitude and phase at ABT, shown across the eastern US for two different times in 2001 (Figure 5) illustrate widely varying temporal and spatial properties of weekday/weekend ozone fluctuation.

Observed and CMAQ diurnal amplitude and phase are compared in Figures 6 and 7. Observed diurnal amplitude at ABT is greater than that of CMAQ. During the 18 years that were modeled, the average diurnal phase difference between observations and CMAQ is zero (cross-correlations between observations and model peak at zero lag). However, there are times (as in Figure 7) when the two are out of phase.

As with seasonal processes, correlations between observed and CMAQ diurnal variation (0.91 and 0.76 at ABT147 and SHN418, respectively), mostly reflect phase differences (Figure 6), while observed/model amplitude correlation (0.79 and 0.41) measure the extent to which the model correctly gauges changes in diurnal forcings (Figure 7). Observation/model agreement was poor at intraday time scales (< 11 hours, R 0.26 and 0.19 at ABT and SHN, respectively), reflecting, in part, the model's inability to simulate stochastic variation like measurement instrument noise.

4. SUMMARY

Wavelet analysis provides frequency specific information about observations and model outputs that can be useful in model evaluation. Differences in the strength (amplitude) between observations and model were illustrated for low-frequency (trend) and intra-day variation, while differences in both strength and timing (phase) were illustrated for seasonal, weekly and diurnal processes. Modulation of seasonal and

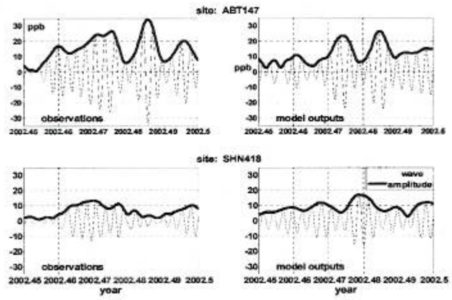

Figure 6. Observed and modeled diurnal variation at ABT and SHN

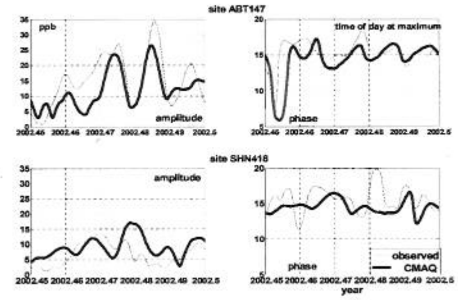

Figure 7. Observed and modeled diurnal amplitude and phase at ABT and SHN

diurnal ozone occurs at low frequencies (three to five years for seasonal and one year for diurnal processes) and can be tied to low frequency variation in meteorological variables. Wavelet analysis of weekly variation can be used to identify spatial/temporal variation in weekday/weekend ozone air quality.

5. ACKNOWLDEGEMENTS

Christian Hogrefe gratefully acknowledges partial support for this work through a research fellowship from the Oak Ridge Institute for Science and Education (ORISE).

6. DISCLAIMER

The model simulations in this paper were supported by National Oceanic and Atmospheric Administration award NAO40AR4310185185, but the paper has not been subjected to its required peer and policy review. Therefore, the statements, findings, conclusions, and recommendations are those of the authors and do not necessarily reflect the views of the sponsoring agency and no official endorsement should be inferred. This work constitutes a contribution to EPA's Air Quality Program. Although it has been reviewed by EPA and approved for publication, it does not necessarily reflect their policies or views.

REFERENCES

Bloomfield, P. 2000. Fourier Analysis of Time Series: An Introduction. Wiley-Interscience; 2nd ed.

CASTNET. 2006. Annual Report. prepared by MACTEC Engineering and Consulting, Inc. for the USEPA Clean Air Markets Division, Washington, D.C.

Hogrefe, C., Lynn, B., Goldberg, R., Rosenzweig, C., Zalewsky, E., Hao, W., Doraiswamy, P., Civerolo K., Ku, J., Sistla, G., and P.L. Kinney. 2009. A combined model–observation approach to estimate historic gridded fields of PM2.5 mass and species concentrations. Atmospheric Environment 43: 2561–2570

Rao, S.T., and I.G. Zurbenko. 1994. "Detecting and tracking changes ozone air quality", J. Air & Waste Manage. Assoc., 44: 1089

Zurbenko, I.G. 1986. The Spectral Analysis of Time Series. North Holland

Zurbenko I., Porter. P.S. 1998. Construction of high resolution wavelets, IEEE Journal of Signal Processing, vol. 65, pp. 315-327.