Analysis of Seasonality and Trends in WRF-CMAQ Modeled $PM_{2.5}$ using Empirical Mode Decomposition

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Scope and Objectives

How well can we capture changes in $PM_{2.5}$ and its speciated components induced by variations in meteorology and/or emissions over a decade?

- Analyze and interpret features embedded in $PM_{2.5}$ observations and model outputs
- Assess the model's ability to reproduce changes/trends in observed $PM_{2.5}$ concentrations
- Propose a new method for model evaluation of $PM_{2.5}$ and its components without any preselection of temporal scales and assumptions of data linearity and stationarity

Data

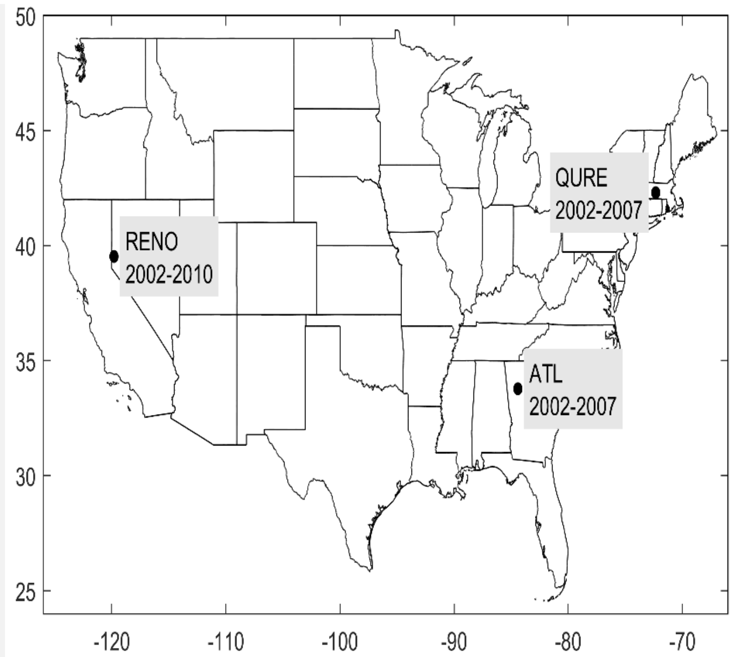
✓ Model simulations

Coupled 2000-2010 **WRF-CMAQ** (vers. 5.0.1) with 36-km grid cells over the USA (Gan et al. 2015; Xing et al. 2013)

✓ Observations:

SO_4, NO_3, NH_4, OC, EC, Cl, and total $PM_{2.5}$ are retrieved from the Chemical Speciation Network (CSN), Interagency Monitoring of Protected Visual Environments (IMPROVE) and SEARCH networks.

3 sites are used to demonstrate the proposed method of evaluation.



Luo et al. 2019; Atm Environ (under review)

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Methodology

Empirical Mode Decomposition (EMD)

Signal x is decomposed to multiple Intrinsic Mode Functions (IMFs) d_i and a residual trend r_k through sifting processes (Huang et al., 1998):

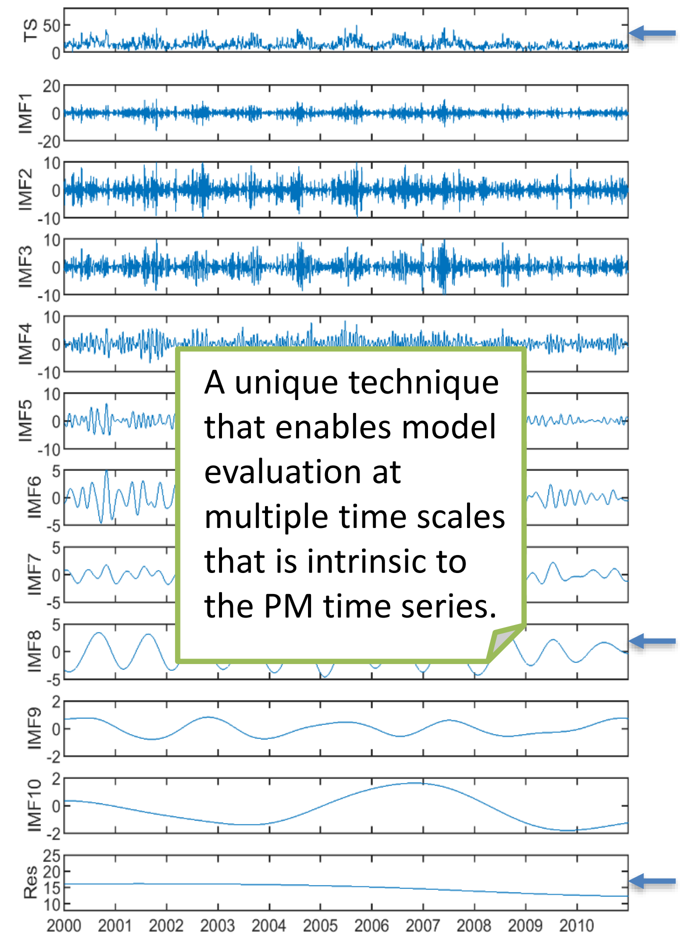
$$x = \sum_{i=1}^{k} d_i + r_k$$

An IMF must satisfy:

1) the number of extrema (maxima and minima) and zero-crossings must be equal or differ at most by one;
2) the local mean, defined as the mean of the upper and lower envelopes, must be zero.

Multiple improvements to address mode mixing as well as other problems are included in the most recent version of Improved Complete Ensemble Empirical Mode Decomposition with Adaptive Noise (Improved CEEMDAN) (Wu and Huang, 2009; Yeh et al., 2010; Torres et al., 2011; Colominas et al., 2014).

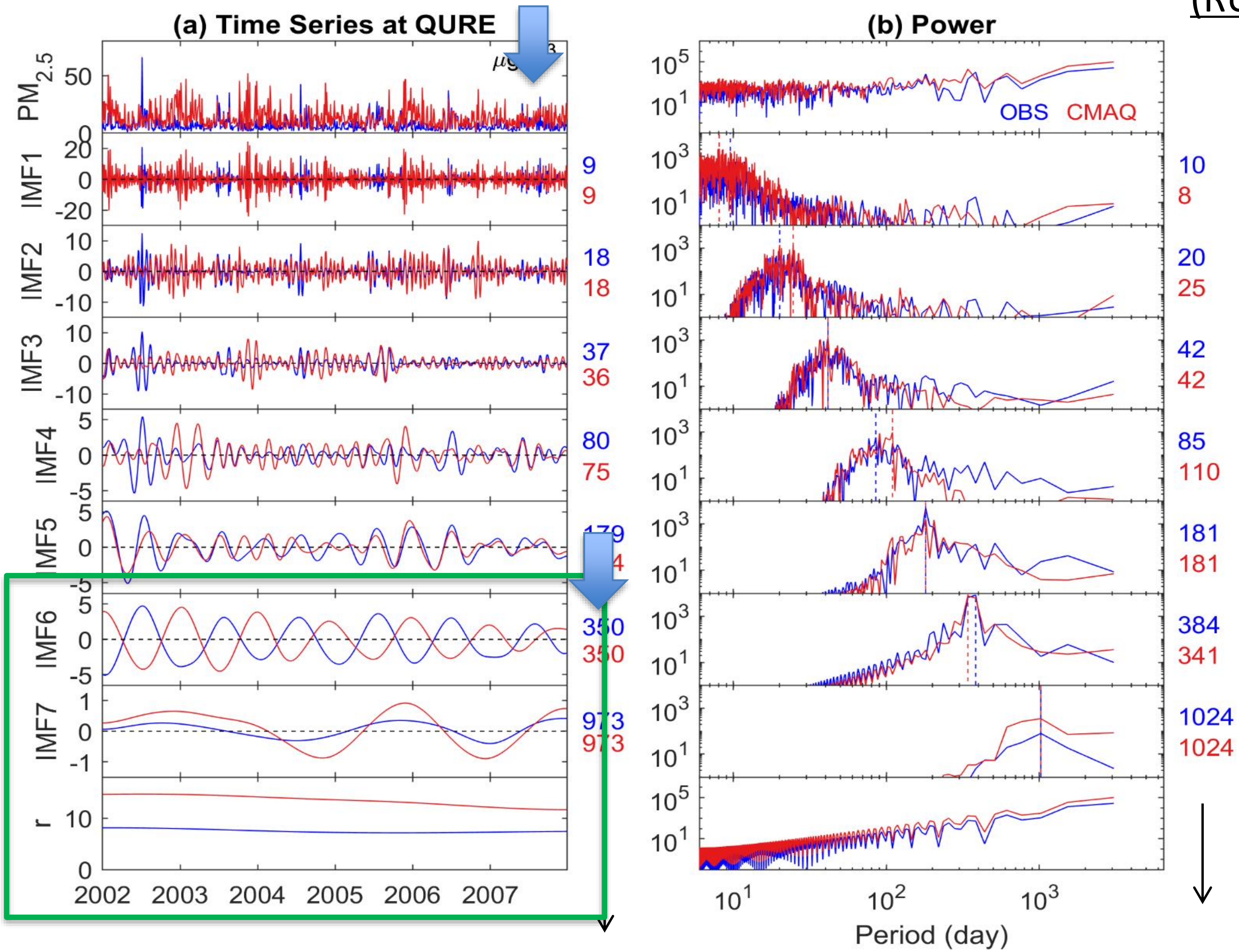
Decomposition of total $PM_{2.5}$ with EMD



Total $PM_{2.5}$ - Quabbin Summit, MA

(RURAL, IMPROVE)

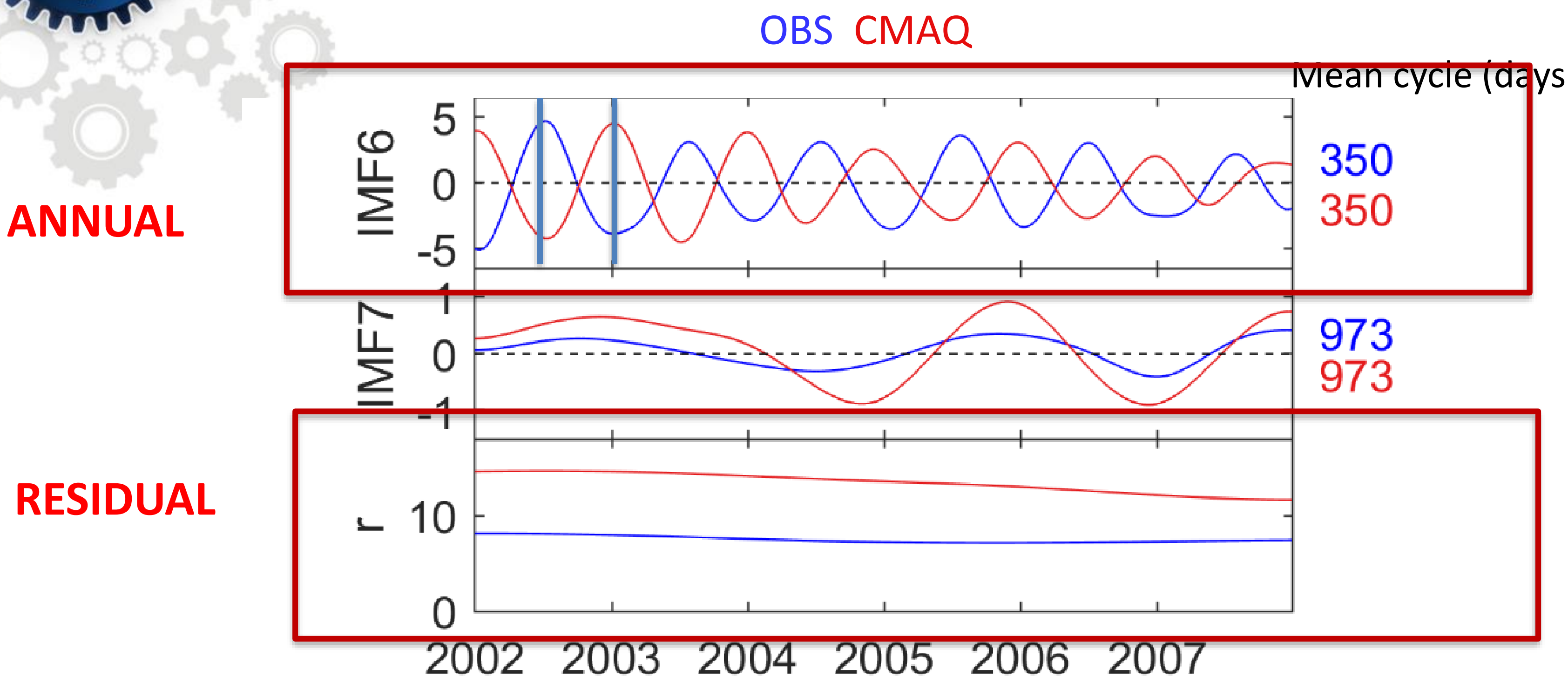
OBS CMAQ



Mean cycle (days)

Peak cycle (days)

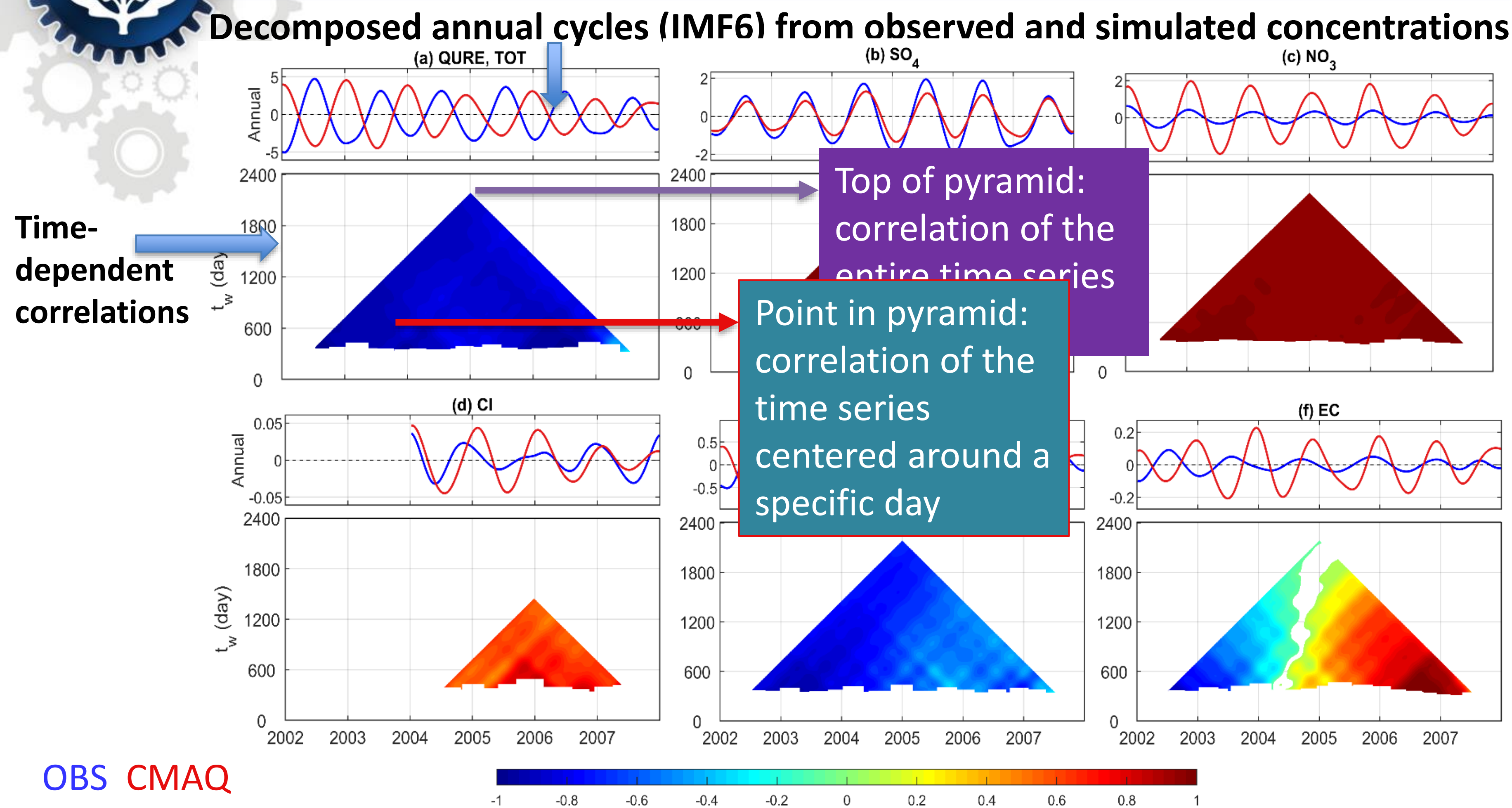
Total $PM_{2.5}$ - Quabbin Summit, MA



- Very clear annual cycles of $PM_{2.5}$ exist in both obs and CMAQ, but they are out of phase by up to six months.

- The residual (trend) indicates overestimation of the magnitude of the trend component by CMAQ; decreasing trend by CMAQ while obs show slight decline

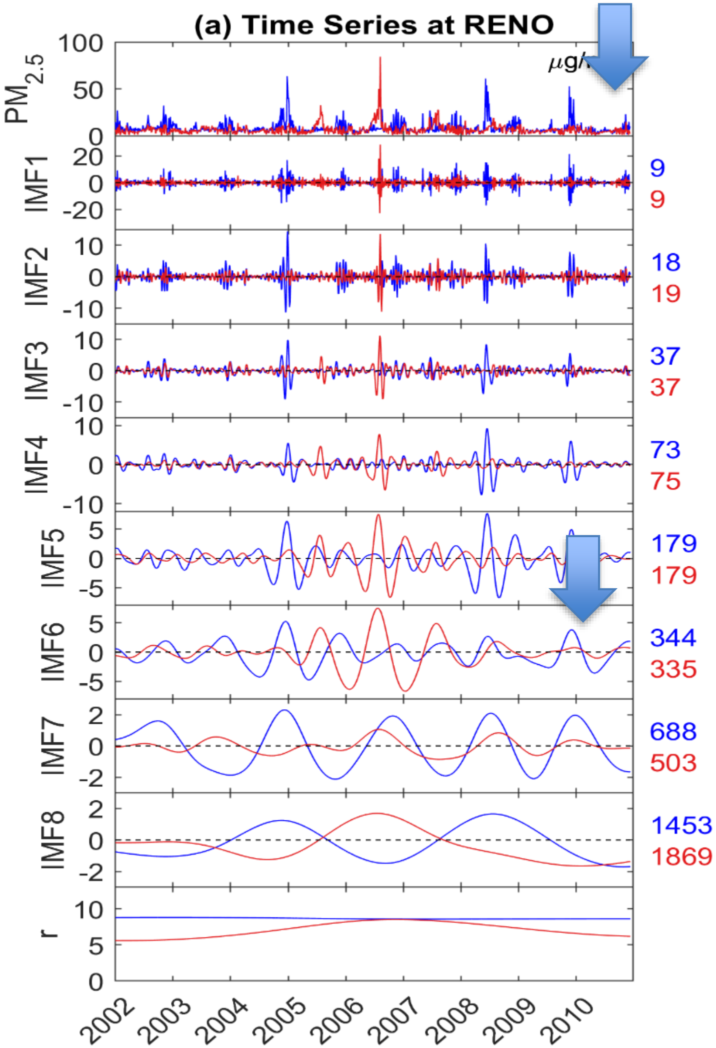
$PM_{2.5}$ components - Quabbin Summit, MA

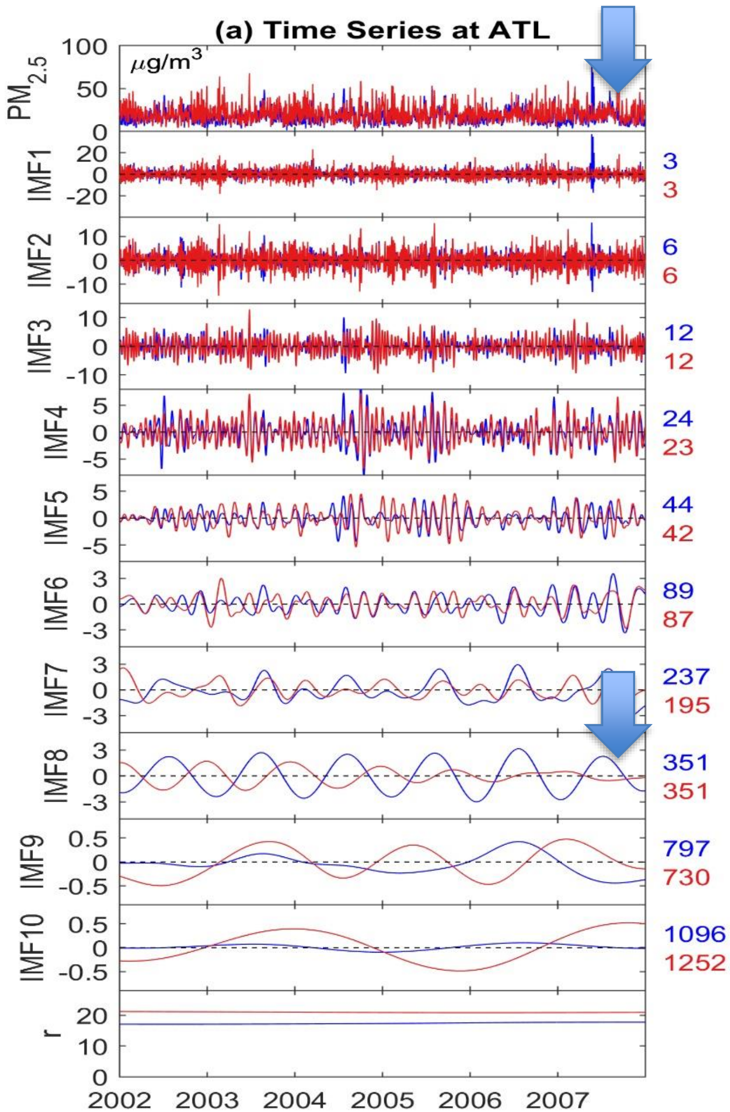


- Overestimated amplitude of NO_3 (4.3 x obs)
- Almost semi-annual shifted OC (-147 days); OC, EC and Cl contribute to the $PM_{2.5}$ shift
- OC directly drives the negative correlations
- EC follows the feature of OC in the first four years

Total $PM_{2.5}$ - Reno, NV and ATL, GA

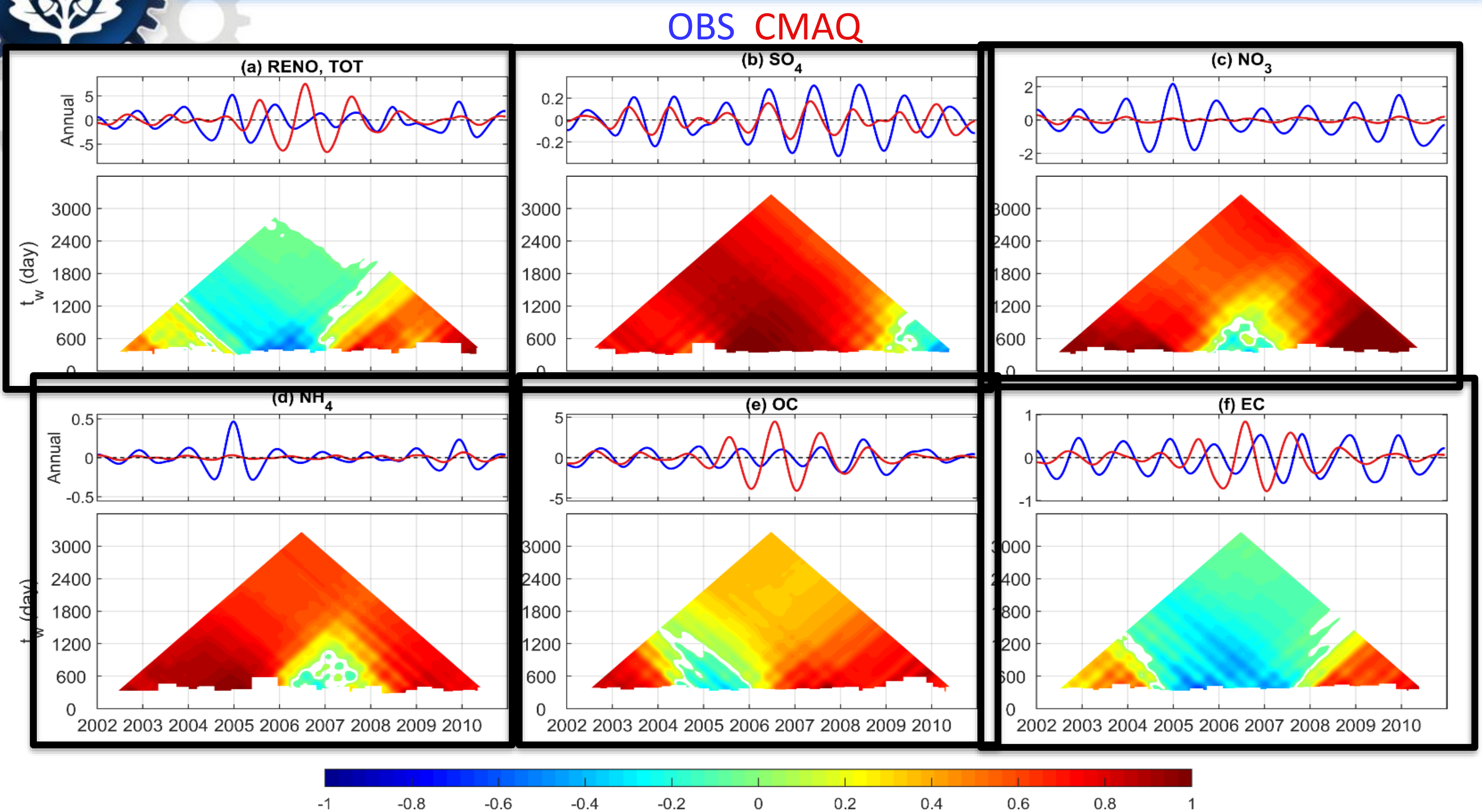
Reno, NV (urban - AQS, CSN) OBS CMAQ ATL, GA (urban - SEARCH)





Mean cycle (days)

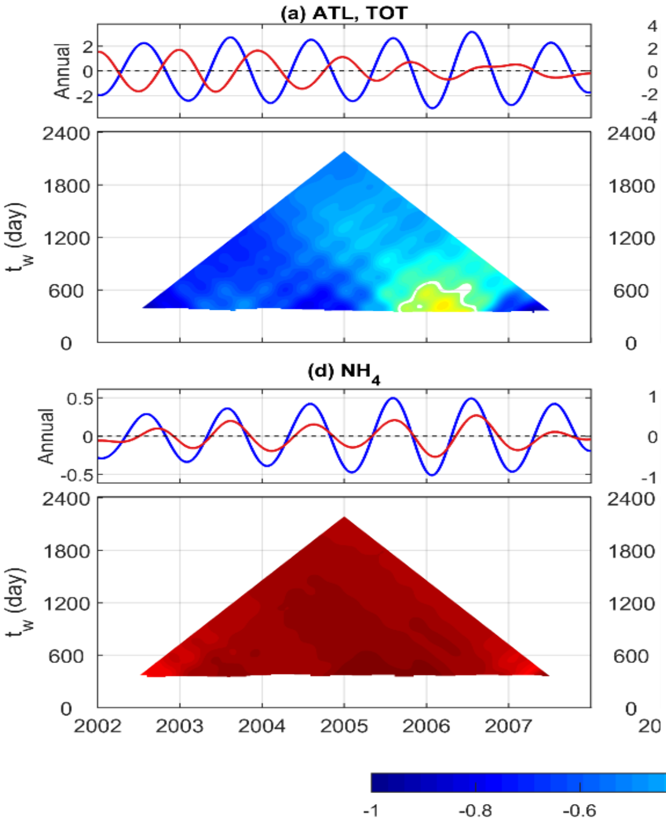
$PM_{2.5}$ components - Reno, NV

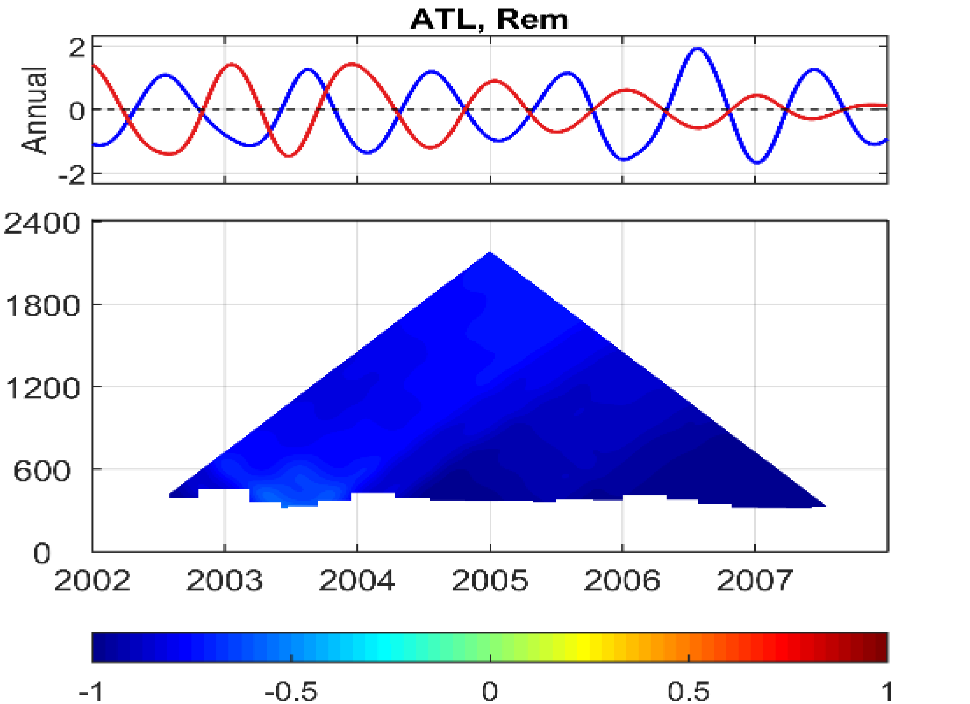


- Site is situated in a wildfire-prone area
- Annual variations for total and speciated $PM_{2.5}$ are largely underestimated
- The modeled phase of SO_4, NO_3, NH_4 and OC agrees with that of observations with few exceptions
- EC mimics the TDIC pyramid of total $PM_{2.5}$, implying the existence of errors in modeled EC that affected the model performance for total $PM_{2.5}$ (potential impact of wildfires)

$PM_{2.5}$ components - ATL, GA

OBS CMAQ





- Simulated total $PM_{2.5}$ shows a shift of several months (132 days)
- Overestimation of NO_3; underestimation of NH_4 and phase shift of EC (54 days)
- Anti-correlated total $PM_{2.5}$ annual cycles cannot be attributed to the available species
- The remaining species clearly played a role in driving the above discrepancies
- Anti-correlation likely due to inaccurate representation of the seasonal variation of the non-C portion of OM in the model version analyzed here that has been updated in more recent releases of CMAQ

Summary

- ✓ The EMD method enables direct comparison of the relative strengths of the various forcings, operating on different time scales, that are embedded in non-linear and non-stationary time series of observed and modeled concentrations
- ✓ Coordinated decomposition and evaluation of total and speciated $PM_{2.5}$ provides a unique opportunity for modelers to assess influences of each $PM_{2.5}$ species to total $PM_{2.5}$ concentration in terms of time shifts for various temporal cycles and the magnitude of each component including the trend
- ✓ At these three sites:
  - The model generally is more capable of simulating the change in the trend than the absolute magnitude of the long-term trend component
  - The magnitude of SO_4 trend components is well represented across all sites
  - The model reproduced the amplitude of the annual cycle for total $PM_{2.5}$, SO_4 and OC
  - The phase difference in the annual cycles for total $PM_{2.5}$, OC and EC reveal a shift of up to half-year
  - More recent versions of CMAQ incorporate many updates to the treatment of organic aerosols that are expected to improve the representation of the seasonal cycle
  - New long-term simulations with CMAQv5.3 are planned for the near future which can be used to confirm this expected improvement

Acknowledgements

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