6.2 ATTAINMENT DEMONSTRATION UNCERTAINTY STEMMING FROM POOR METEOROLOGICAL MODEL PERFORMANCE

Saffet Tanrikulu,[1*] Scott Beaver,[1] Ahmet Palazoglu,[2] Angadh Singh[2]

[1]Bay Area Air Quality Management District, San Francisco, CA
[2]University of California, Dept. Chemical Engineering and Materials Science, Davis, CA

1. INTRODUCTION

Several air quality models have been applied over central California for decades, originally for modeling ozone, and more recently for modeling fine particulate matter ($PM_{2.5}$) and air toxics. They all consistently underestimated pollutant levels on days for which the highest pollutant levels were observed. Days having moderate pollutant levels, however, were generally simulated reasonably. Air pollution agencies and stakeholders have rigorously investigated causes of this underestimation problem, mostly focusing on meteorological and emissions inputs.

Among the meteorological models used for preparing inputs, the MM5 model consistently performed the best. Therefore, it was a natural choice for preparing meteorological inputs. Emission estimates have been significantly improved through source testing and field studies. Despite these significant efforts, the root cause of the underestimation problem has not been discovered until recently.

In a recent study, the MM5-CAMx couple was applied over central California to simulate smoke from household wood burning, a directly emitted and inert type of $PM_{2.5}$. Chemistry was turned off in CAMx. Identical wood burning emissions were simulated for every day of a 3-month “wood burning” season. Simulated $PM_{2.5}$ concentrations were compared against observed organic carbon fractions representing $PM_{2.5}$ mostly from wood burning. The same systematic air quality underestimation occurred. The model accurately estimated low to moderate wood smoke levels. But it strongly underestimated the high wood smoke levels for the episodic, strongly conducive periods. Simulated levels for strongly conducive days were often even lower than for moderately conducive days. This information suggested that MM5 performance, as opposed to emissions, was causing the underestimation.

In a separate study, Beaver et al. (2010) found that operational evaluations of the MM5-generated meteorological fields typically indicate similar statistical performance of MM5 across days with moderate to high observed pollutant levels. Therefore, deficiencies in MM5 for high pollutant days are undetected using this type of empirical evaluation. They demonstrated that a pattern-based diagnostic evaluation of MM5 is more suitable for detecting deficiencies in MM5-generated winds as well as other meteorological parameters during high pollutant days.

In this study, we investigated uncertainty introduced to air quality model sensitivity due to underestimation of pollutant concentrations. Because improving model performance for days with elevated pollutant levels may require conducting lengthy comprehensive research, it is important to follow the technique presented in this paper to assess the uncertainty introduced to State Implementation Plans. Below, we demonstrate the uncertainty for a winter particulate matter episode using the MM5-CMAQ couple; however, we believe that this type of problem is ubiquitous and impacts other seasons, pollutants and areas. Our method could be an important tool for regulatory agencies until the root cause of the underestimation problem is resolved.

2. METHOD

The study proceeds in two phases: a pattern-based evaluation of coupled MM5-CMAQ performance, followed by a numerical experiment.

The pattern-based evaluation technique is described by Beaver et al. (2010) and details can be found therein. In short, *cluster analysis* is applied to meteorological observations to identify a set of weather patterns associated with distinct air pollution characteristics. Next, the actual conditions for each day within the simulation period are labeled as one of these identified weather patterns. *Classification* is then applied to simulated meteorological fields. The simulated conditions for each day within the simulation period are labeled using the same set of observation-derived weather patterns. A comparison is made between labels for the observed and simulated weather patterns. For a given day, a match between the observation-based label and the simulation-based label implies that the simulated fields are accurate. Mismatches indicate days having poorly simulated fields. Pattern matching is used to determine which, if any, day with accurately simulated fields is most representative of each poorly simulated day.

The numerical experiment involves CMAQ simulations with original and substituted meteorological inputs. The methodology requires that MM5 reasonably simulates the meteorological fields for at least one representative day during an episode of interest so that these fields can be used as

---

* *Corresponding author address:* Saffet Tanrikulu, Bay Area Air Quality Management District, 939 Ellis St, San Francisco, CA 94109; e-mail: stanrikulu@baaqmd.gov

substitutes for the mismatching days' original meteorological inputs. Simulating with the representative (substituted) meteorological fields should, on average over the duration of the episode, improve air quality model performance relative to using the original, biased meteorological fields.

The numerical experiment comprises four simulations in total. Two use the original meteorological fields, and two use the substituted meteorological fields. For each set of meteorological inputs, a base case and a sensitivity simulation (having reduced anthropogenic emissions) are conducted. In terms of uncertainty, model response to emission reduction was examined in both the absolute and relative senses.

3. MODEL SETUP

The air quality modeling domain included all low-lying areas within central California over which elevated winter $PM_{2.5}$ levels were monitored (area shown in Figure 1). The simulation period was 25 December 2000 through 6 January 2001, spanning 13 consecutive days. This period was selected because it corresponded to an intensive operational period during which special data were collected as part of the California Regional Particulate Air Quality Study (CRPAQS).

The MM5 model was applied with three nested domains with 36-, 12-, and 4-km horizontal resolutions. The CMAQ model was applied with 185×185 grid cells and 4 km horizontal resolution, covering the innermost domain of MM5. There were 30 MM5 and 15 CMAQ vertical layers. The bottom layers of both models were approximately 22 m thick. Initial and boundary conditions for CMAQ were obtained from specialized measurements of CRPAQS.

Emissions were prepared mostly from an annual inventory for base year 2000 supplied by the California Air Resources Board (ARB). The San Francisco Bay Area portion of this inventory was replaced by the BAAQMD planning inventory. Biogenic emissions were prepared using climatologically representative meteorological data. Emissions were spatially, temporally and chemically allocated using the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System.

4. RESULTS AND DISCUSSION

A meteorological cluster analysis was conducted to identify winter-season weather patterns associated with distinct $PM_{2.5}$ characteristics (Beaver et al., 2010B). The clustering was conducted for the months November through March of years 1996-2007 based on Bay Area measurements. Two important weather patterns were identified that are relevant to this study (Figure 1). These patterns are named R1 and R2, where the "R" indicates the presence of an aloft ridge of high pressure over central California. Pattern R1 was pre-episodic in nature. It exhibited moderate wind speeds and moderate $PM_{2.5}$ levels. Pattern R2 was episodic in nature. It exhibited low wind speeds and high $PM_{2.5}$ levels. There were 219 and 422 days, respectively, assigned to patterns R1 and R2. These patterns were highly significant and representative of typical pre-episodic and episodic conditions, respectively.

Cluster labels for the observed weather patterns and also observed $PM_{2.5}$ levels during the simulation period (25 December 2000 through 6 January 2001) are shown in Figure 2. The first day, 25 December, was assigned to pattern R1. It had moderate Bay Area $PM_{2.5}$ levels at around 20 $\mu g/m^3$. All other days in the simulation period were assigned to pattern R2. All of the days assigned to R2 had exceedances of the 24-hour average National Ambient Air Quality Standard (NAAQS) of 35 $\mu g/m^3$ in the Bay Area. $PM_{2.5}$ episodes typically involved some buildup. As such, the first R2 day, 26 December, exhibited moderately high $PM_{2.5}$ levels that were near the exceedance threshold. The subsequent days for which the R2 pattern persisted exhibited some of the highest Bay Area $PM_{2.5}$ levels on record, approaching 60 $\mu g/m^3$.

Classification of the MM5-generated meteorological fields into the observation-derived weather patterns was then conducted. Some additional labels were defined for days that did not cleanly fit into a single observation-derived weather pattern (cluster). Pattern R* was a hybrid sharing properties of both R1 and R2. Pattern R+ exhibited some precipitation into the evening hours, whereas the other patterns were dry. R1 and R*, which share some properties with R1, were less conducive to $PM_{2.5}$ buildup than R2 because their wind speeds were higher and their low-level air flow patterns were deeper. R+ was less conducive than R2 because its precipitation was associated with $PM_{2.5}$ wet deposition and its cloudy conditions likely slowed photochemical formation of secondary $PM_{2.5}$.

Meteorological regime classifications and simulated $PM_{2.5}$ levels based on the original MM5-generated meteorological fields and the base case emissions inventory are colored red in Figure 2. Of the 13 days in the simulation period, only 2 were simulated accurately by MM5. The first day, 25 December, had meteorological conditions accurately simulated as R1. $PM_{2.5}$ levels were likewise accurately simulated as moderate. Day 5 January also had meteorological conditions accurately simulated as R2. For all other days, mismatches occurred between the simulated and observed weather pattern. Observed conditions were episodic (R2), but simulated conditions were less strongly conducive to high $PM_{2.5}$ levels. Accordingly, the CMAQ-simulated $PM_{2.5}$ levels were underestimated for all of these mismatching days. The single day with accurately simulated (matching) meteorology, 5 January, also exhibited underestimated simulated $PM_{2.5}$ levels. Simulated $PM_{2.5}$ levels for this lone matching R2 day were underestimated because multiple consecutive R2 days were typically required for high $PM_{2.5}$ levels to develop. In summary, $PM_{2.5}$ levels for the exceedance days were consistently underestimated by CMAQ because the meteorological fields simulated by MM5 were mostly insufficiently conducive to $PM_{2.5}$ buildup.

Day 5 January exhibited the only accurately simulated R2 meteorological conditions during the exceedance period. The episode occurred under persisting conditions for which the large-scale pressure gradients and surface winds were similar for all days. Therefore, the accurately simulated meteorological fields for 5 January were deemed representative of the other, improperly simulated R2 days. A modified simulation was then conducted with meteorological fields from 5 January substituted for each day in the period 26 December through 6 January. The original meteorological fields were retained for moderately conducive matching day 25 December (assigned to R1).

Meteorological regime classifications and simulated $PM_{2.5}$ levels based on substituted meteorological fields and base case emissions are colored blue in Figure 2. (The repeated R2 pattern for this model run represents the 5 January meteorological fields substituted for the other days observed as R2.) Simulating the same meteorological fields throughout the exceedance period resulted in simulated $PM_{2.5}$ levels that increased pseudo-exponentially from an initial, moderate level to high levels after about 2-3 days of buildup. The substitution of the representative, accurately simulated meteorological fields produced $PM_{2.5}$ levels having similar magnitude as the observations. In summary, substituting the best-matching meteorological fields for the mismatching days dramatically improved CMAQ base case performance during the episode.

Sensitivity runs, using both the original and substituted meteorological fields, were conducted. The emissions inventory simulated in the sensitivity runs had a 20% across-the-board reduction for all anthropogenic emissions relative to the base case inventory. Figure 3 shows the sensitivity estimates for $PM_{2.5}$ level, expressed as both a difference (c_{sens}^{m} - c_{base}^{m}) and as a relative response factor (RRF). Expressed as a difference, the $PM_{2.5}$ levels for the runs with substituted meteorology were significantly more sensitive to the same change in emissions. As indicated in Figure 2, the modified simulation produced base case $PM_{2.5}$ levels that were roughly twice as large (around 60 $\mu g/m^3$) as for the original simulation (around 30 $\mu g/m^3$). Correspondingly, reductions in $PM_{2.5}$ levels in the sensitivity runs were around twice as large (top right panel of Figure 3, around 6-10 $\mu g/m^3$) as for the original simulation (top left panel of Figure 3, around 2-6 $\mu g/m^3$) at a given location.

Expressed as RRF, the variability in the $PM_{2.5}$ sensitivities between the models having the original and substituted meteorological fields exhibited a complex spatial distribution. In the southern Bay Area around San Jose, RRF^{orig} was 0.76 and RRF^{mod} was 0.83. Thus, the substituted meteorology resulted in an RRF value that was around 0.07 larger (less benefit) in the southern Bay Area. Around Sacramento, the impact of the substituted meteorology was to decrease the RRF estimate by 0.03 (more benefit) from RRF^{orig} of 0.83 to RRF^{mod} of 0.80. In the San Joaquin Valley (SJV; large inland valley including Fresno and Bakersfield), the substituted meteorology had a relatively minor impact on the RRF estimates.

5. CONCLOUSIONS

The RRF workaround specified in the US EPA guidelines may be inapplicable when systematically poor MM5 performance results in seriously degraded photochemical air quality model performance. RRF may be overestimated or underestimated, depending on location.

The uncertainties for RRF presented here are numerically small. When applied to observation-derived design values as part of an attainment demonstration, however, the uncertainties could have serious impacts on air quality planning efforts. At San Jose, the RRF uncertainty of 0.07 multiplied by the current design value of 36 $\mu g/m^3$ corresponds to over 2 $\mu g/m^3$ overestimated benefit of the 20% emissions reductions. This level of uncertainty could result in an inaccurate attainment demonstration for an already heavily regulated area in which additional emissions controls are costly.

Regional differences in RRF uncertainties may reflect the region-specific manner in which the pattern-based meteorological analysis was conducted. The pattern-based meteorological analysis was conducted based on the Bay Area measurements. The low level of variability for RRF in the SJV likely resulted because weather patterns R1 and R2 were least distinguishable for this region (see Figure 1). These patterns, however, may not be optimal for explaining meteorological influences on $PM_{2.5}$ episodes in the SJV. In the future, we plan to repeat the described RRF uncertainty analysis to focus on other regions such as around Sacramento and the SJV.

REFERENCES

Beaver, S., Tanrikulu, S., Palazoglu, A., Singh, A., Soong, T.Z., Jia, Y., Tran, C., Ainslie, B., Steyn, D., 2010A. Pattern-based evaluation of coupled meteorological and air quality models. *Journal of Applied Meteorology and Climatology*, **49**, 2077-91.

Beaver, S., Palazoglu, A., Singh, A., Soong, T.Z., Tanrikulu, S., 2010B. Identification of weather patterns impacting 24-h fine particulate matter pollution. *Atmospheric Environment*, **44**, 1761-71.

Gilliam, R.C., C. Hogrefe, S.T. Rao, 2006: New methods for evaluating meteorological models used in air quality applications. *Atmos. Environ*., **40**, 5073-5086.

Beaver S., Tanrikulu, S., Tran, C., Soong, S.-T., Jia, Y., Rogers, R., Deng, A., Stauffer, D., 2011. Fine Particulate Matter Modeling in Central California, Part II: Application of the Community Multiscale Air Quality Model. AMS 2011 Annual Meeting, 13th Conference on Atmospheric Chemistry, Seattle, WA.

US EPA, 2007. Guidance on the use of models and other analyses for demonstrating attainment of air quality goals for ozone, $PM_{2.5}$, and regional haze. Publication EPA-454/B-07-002. 253 pp.

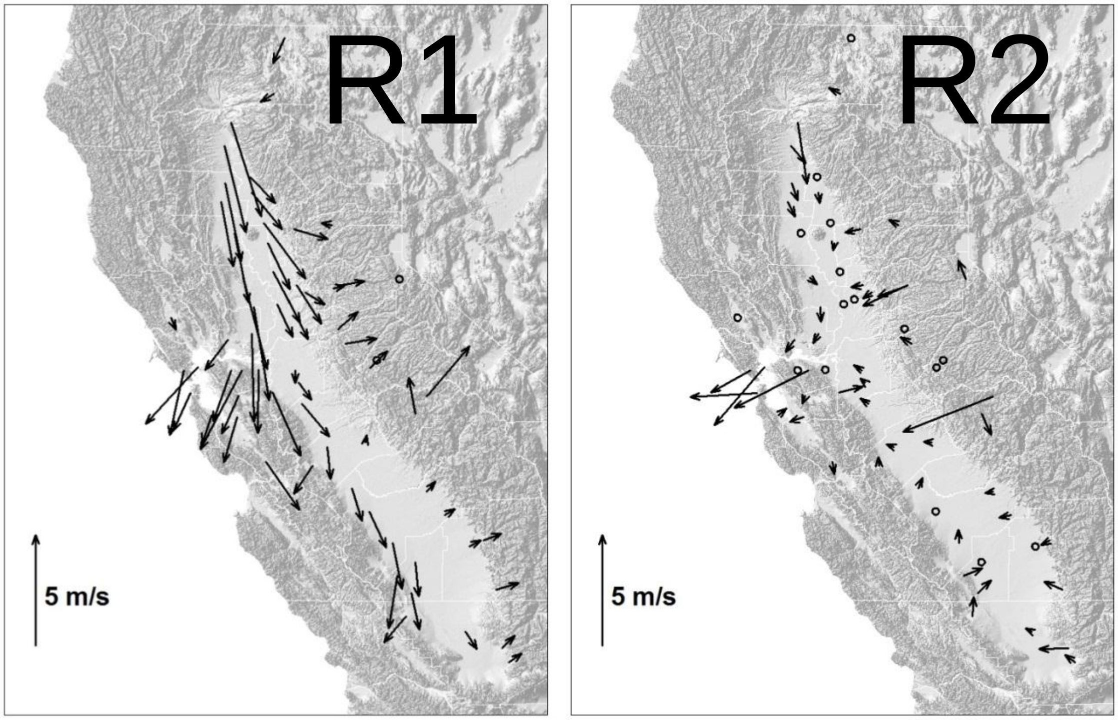

Figure 1. Mean observed 0900 PST surface air flow patterns for two important weather patterns impacting central California winter $PM_{2.5}$ characteristics. Arrows point along direction of wind with tails at weather station positions. Circles indicate calm winds. Pattern R1 is pre-episodic and typically exhibited moderate $PM_{2.5}$ levels. Pattern R2 is episodic and typically exhibited high $PM_{2.5}$ levels.

R1	R2	R2	R2	R2	R2	R2	R2	R2	R2	R2	R2	R2
R1	R1	R1	R1	R*	R*	R1	R1	R1	R1	R*	R2	R+
R1	R2	R2	R2	R2	R2	R2	R2	R2	R2	R2	R2	R2

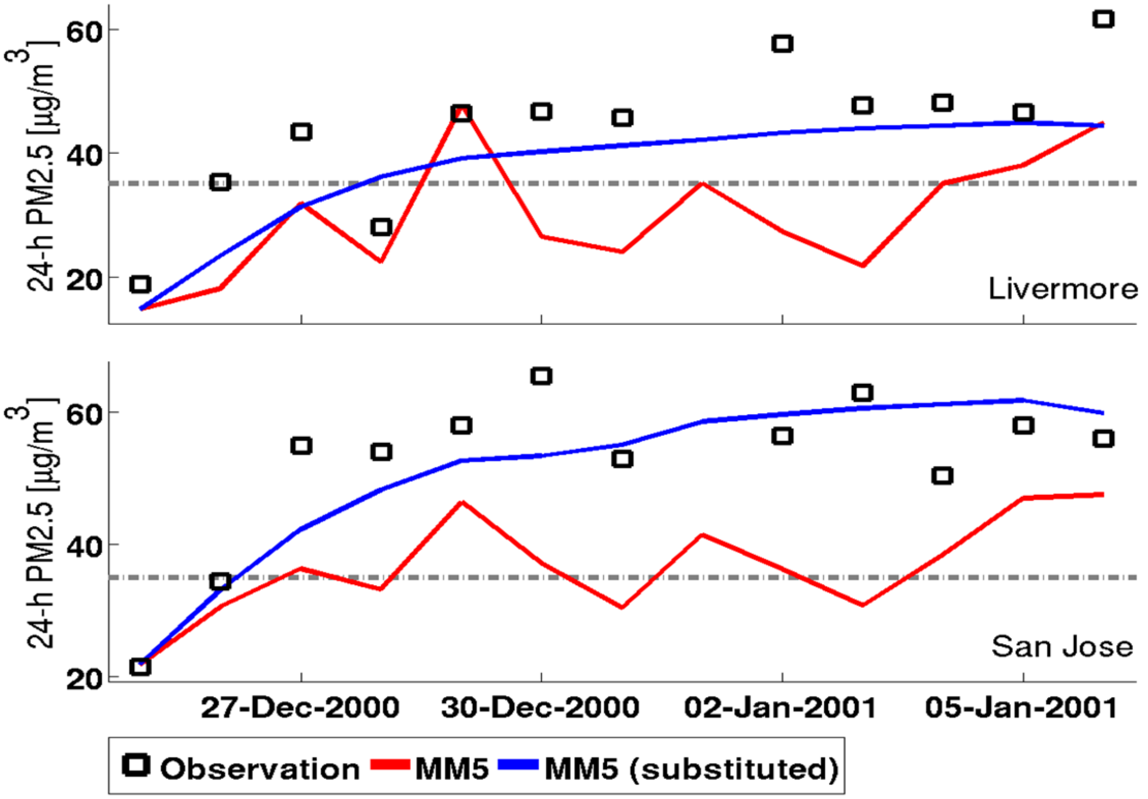

Figure 2. Top: Daily labels for weather pattern assignments for observation (black), simulation with original meteorology (red), and simulation with substituted meteorology (blue). Pattern R* is a hybrid sharing properties of both R1 and R2. Pattern R+ exhibited precipitation, whereas the other patterns were dry. For the simulation with substituted meteorology (blue), all R2 labels correspond to the 5 January meteorological fields from the original MM5 simulation that were replicated from the period 26 December through 6 January.

Bottom: Time series for 24-h $PM_{2.5}$ levels from observation (black squares), simulation with original meteorology (red line), and simulation with substituted meteorology (blue line) for two Bay Area monitoring locations at Livermore and San Jose. Dashed horizontal gray lines at 35 µg/m^3 indicate the 24-h $PM_{2.5}$ NAAQS exceedance threshold.

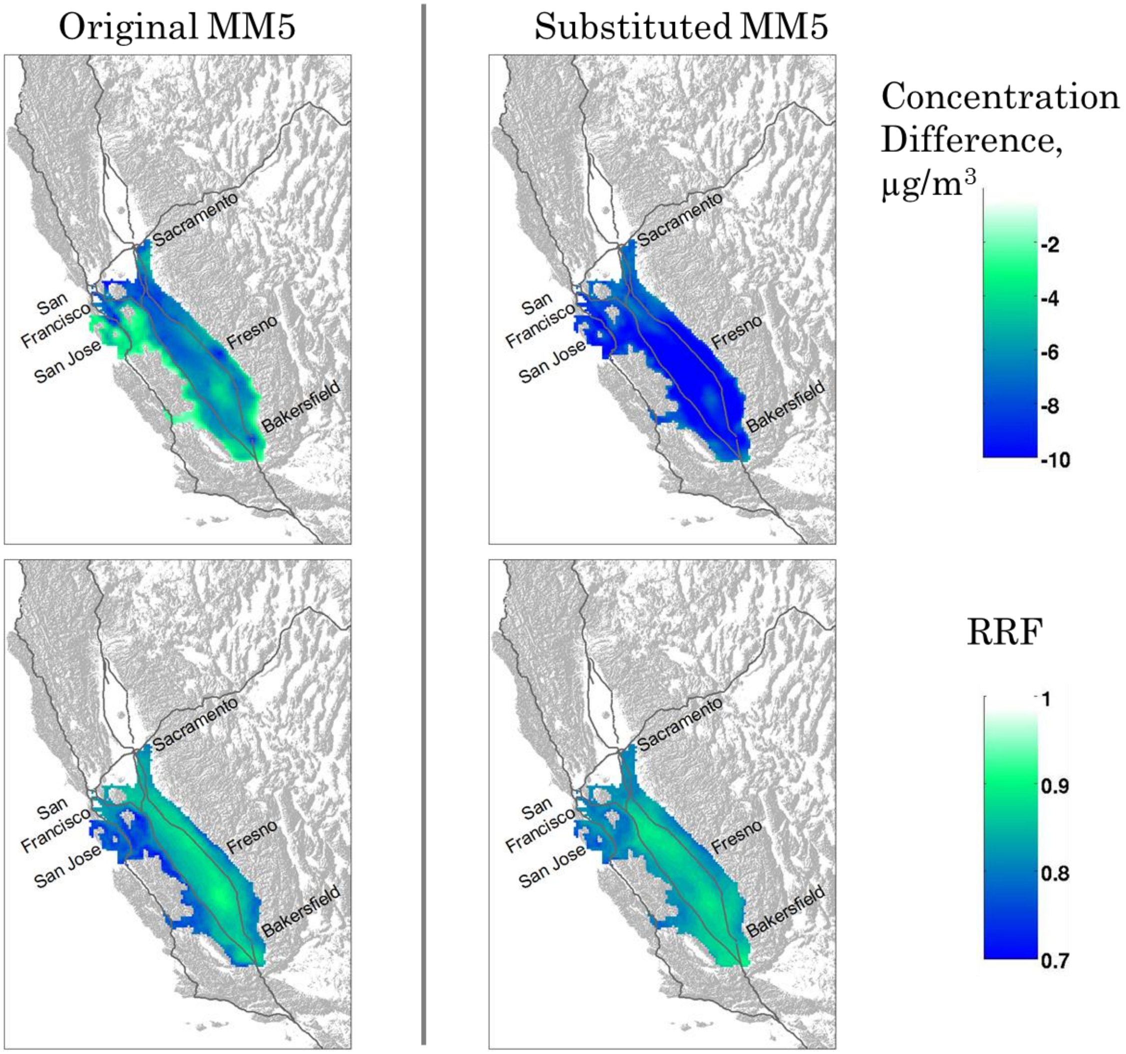

Figure 3. Model $PM_{2.5}$ sensitivity run results for 20% across-the-board reductions for all anthropogenic emissions relative to base case inventory. Sensitivities are expressed as concentration difference (top row) and RRF (bottom row) for simulations with original MM5-generated meteorology (left column) and substituted meteorology (right column). Lower values (toward blue end of color scale) indicate greater benefits of the emissions reductions.