# INVESTIGATING CAUSES OF CMAQ UNDER-PREDICTIONS OF SEA SALT AEROSOL IN THE SAN FRANCISCO BAY AREA

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## 1. INTRODUCTION

To study health impacts, we used CMAQ to make year-round PM2.5 simulations over Central California for 2012. A comparison of the simulated PM2.5 with observations in the San Francisco Bay Area (SFBA) showed under-prediction of PM2.5 during summer, particularly May. This paper presents an analysis of possible causes of the under-prediction and a suggested remedy for the problem.

## 2. METEOROLOGY MODEL

We used the WRF model to generate the meteorological data input to CMAQ. The WRF model used a triple nested domain (Fig. 1) with 36km-12km-4km grid resolutions. Domain 3 is centered on Central California. The year-round simulations actually cover the 2nd through the 15th for February to November, and the 2nd to the end of the month for January and December. PM2.5 exceedances in the SFBA happen mostly in January and December so we extended the simulation periods for these two months.

## 3. AIR QUALITY MODEL

For most of the air quality simulations, we used the CMAQ model version 5.0.2 and saprc99-ae5 chemical mechanisms. A few runs were made using CMAQ version 5.1 and saprc07-ae6 chemical mechanisms for comparison purposes. Domain 3 with 4 km grid resolution was used for the majority of the air quality simulations. Lateral boundary conditions for the most model runs were derived from MOZART data. A few runs used the profile boundary conditions (EPA-derived constant profiles for gases and PM) for reasons to be explained later.

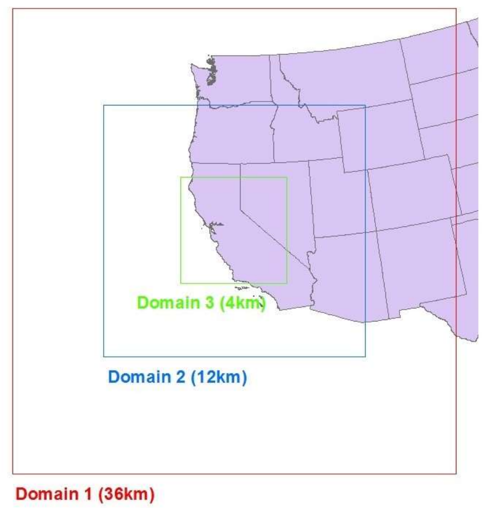


Fig. 1 Triple nested domain used in the WRF simulations.

## 4. EMISSIONS

We prepared emissions for areas within the jurisdiction of the Bay Area Air Quality Management District (BAAQMD). For areas outside of the SFBA, we used the emissions generated by the California Air Resources Board (CARB).

## 5. RESULTS OF THE BASE CASE SIMULATION

Fig. 2 shows the daily observed and simulated PM2.5, averaged over all stations in the SFBA. There is a clear pattern of over-prediction of PM2.5 during the winter months and under-prediction during the summer months. The under-prediction is especially noticeable for May, in which the observations showed a systematic gradual increase in PM2.5 from the beginning of the month to the 9th, followed by a gradual decrease in PM2.5 toward the 15th of the month.

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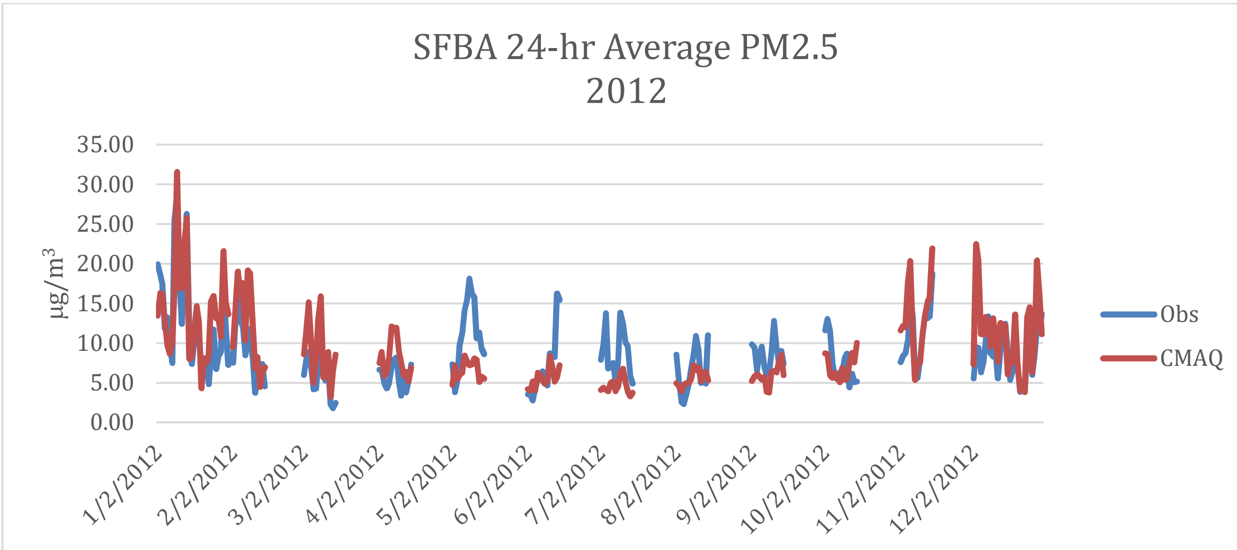


Fig. 2 Daily observed and simulated PM2.5, averaged over all stations in the SFBA.

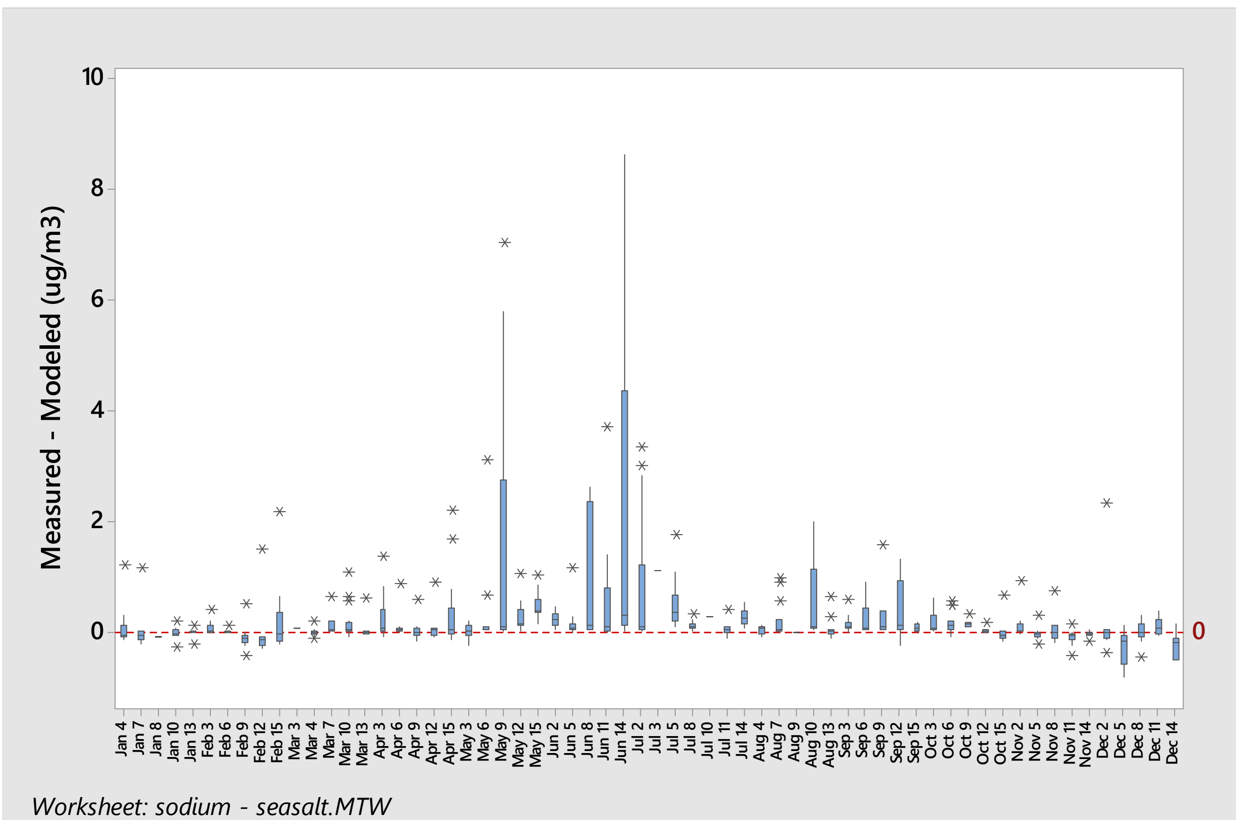


Fig. 3 Daily differences between measured and simulated sea salt averaged over all California stations.

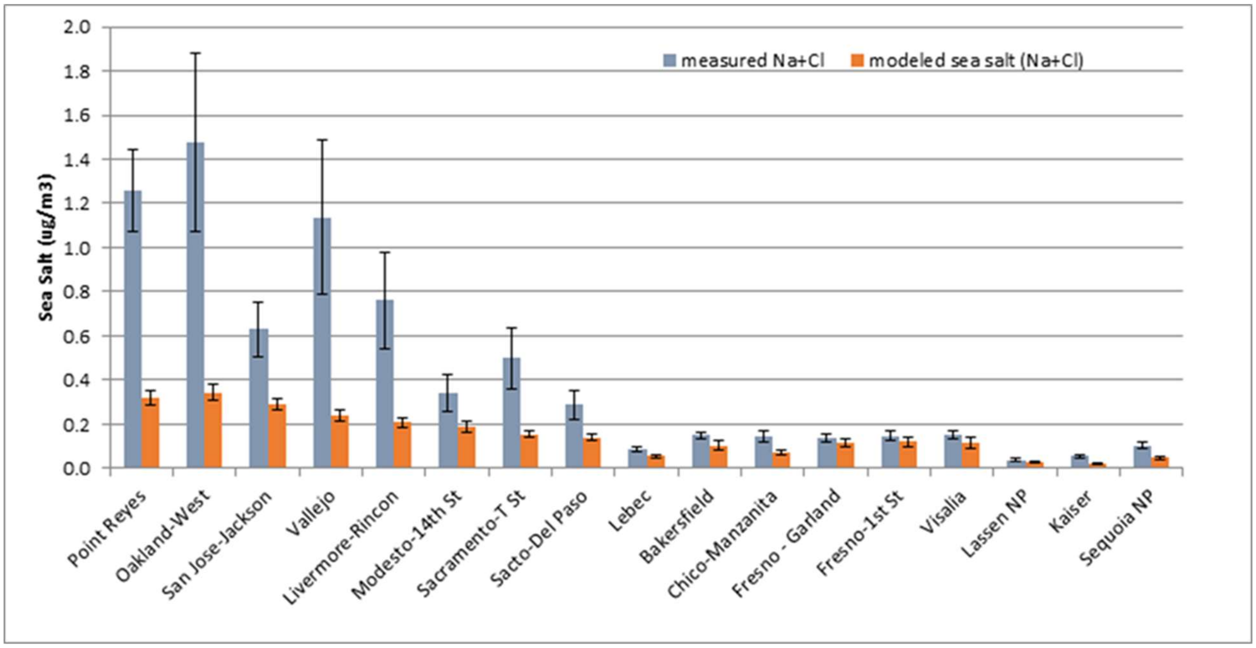


Fig. 4 Observed and simulated annual mean sea salt at selected stations

## 6. ANALYSIS OF SEA SALT PREDICTIONS

We compared simulated PM2.5 with speciated observation data in order to understand the cause of under-prediction of PM2.5 during summer. Fig. 3 shows boxplots of the daily differences between measured and simulated sea salt averaged over all California stations. The speciated data are available every six days for most stations. For a few stations, the speciated data are available every three days.

During winter months, the observed and simulated sea salts are comparable; however, for many summer days, observed sea salt is considerably larger than the simulated values. For May 9, the day of special emphasis in this paper, 50% of the observed sea salt is 3 $\mu g/m^3$ larger than the simulated values. The observed sea salt at one station is 7 $\mu g/m^3$ larger than the simulated value.

Fig. 4 shows the observed and simulated annual mean sea salt concentration at selected stations. The arrangement of the stations is based on distance from the coast. It is obvious that the stations close to the coast have larger sea salt concentrations. San Jose has less sea salt than Vallejo and Livermore because the path of the prevailing summertime onshore wind crosses Vallejo and Livermore on the way toward the Central Valley instead of passing through San Jose.

The CMAQ model under-predicted sea salt at all stations. The under-prediction is most severe for stations near the coast, which include all stations in the SFBA. The observed annual average sea salt is 2-5 times the simulated values. The problem of under-prediction in the Central Valley is much smaller.

At Point Reyes and West Oakland, the CMAQ model under-predicted the daily average sea salt almost every day (Figs. 5a and 5b). The under-prediction is much larger in the summer than in the other months. The daily observed sea salt can be as large as 10 times the simulated value. It could indicate some difficulty for the sea salt algorithm in CMAQ when applied to California and the eastern Pacific, where the wind during summer is particularly strong due to the intense Pacific high.

In Fig. 5, the simulated sea salt does not change significantly from summer to winter while the observed sea salt has maxima in May and June. Also, sea salt at West Oakland has much larger summer-winter differences than at Point Reyes. This is understandable since Point Reyes is right by the ocean and is affected by the ocean-generated sea salt year round. West Oakland is on the east side of San Francisco Bay, and the observed sea salt at this location is governed by the prevailing wind as much as the ocean-generated sea salt. During May and June, the onshore wind is particularly strong and it can easily transport ocean sea salt to this station. During winter months, offshore wind prevails and West Oakland has much less ocean sea salt.

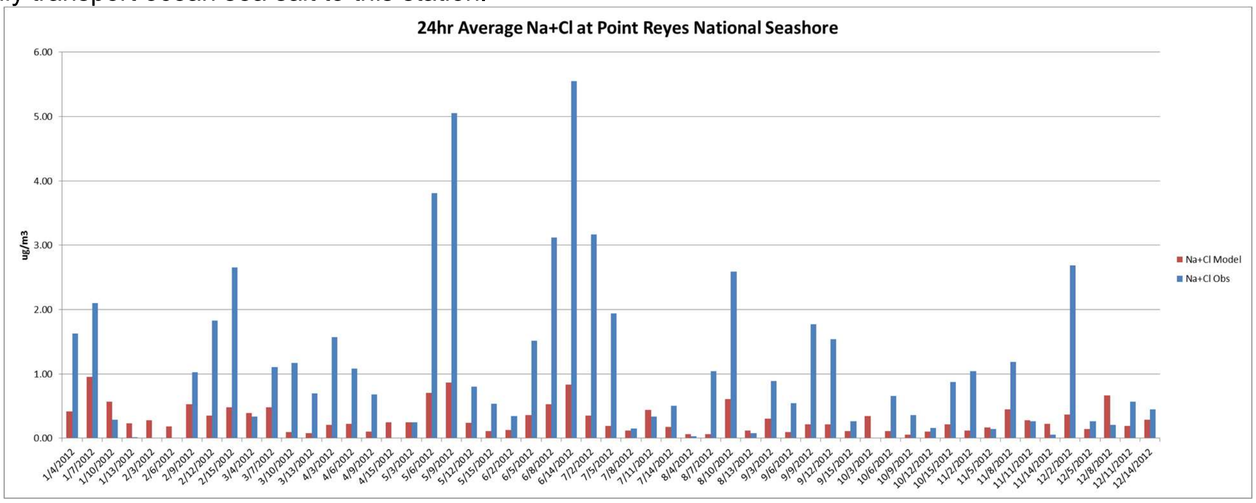


Fig. 5a Daily average sea salt at Point Reyes station

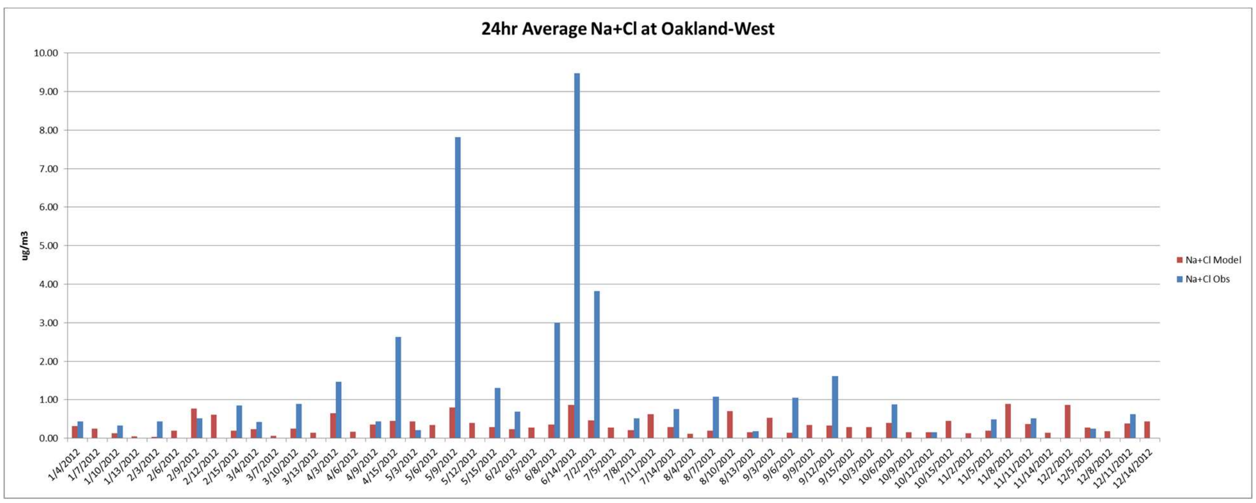


Fig. 5b Daily average sea salt at West Oakland station

## 7. SEA SALT GENERATION

Domain 3, over which most of our simulations were made, covers a limited ocean area. In order to understand the generation of sea salt in CMAQ, we did a few runs using domain 1, which extends 1000 miles over the Pacific Ocean from the California coast. For these runs, we set anthropogenic emissions to zero in the areas outside of domain 3. We also used the profile lateral boundary conditions. These assumptions should not cause a problem for the purpose of studying sea salt generation over the ocean.

An example of the WRF-simulated winds on May 9 is shown in Fig. 6. This is the day with high observed sea salt in the SFBA. The wind is especially strong over the ocean, from the northern California coast to the southwestern model boundary. This is apparently a high sea salt generation area.

The concurrent sea salt concentrations are shown in Fig. 7. The area of maximum sea salt is several hundred km south of the area of strong wind and it is the area of sea salt accumulation. The simulated maximum sea salt is located by the coast south of the SFBA and has a magnitude of 2.3 $\mu g/m^3$. This value is much less than the daily average sea salt on May 9 at either Point Reyes or West Oakland (Fig. 5). We can also see sea salt intrusion into the SFBA in Fig. 7. The concentration, though, is less than 1 $\mu g/m^3$.

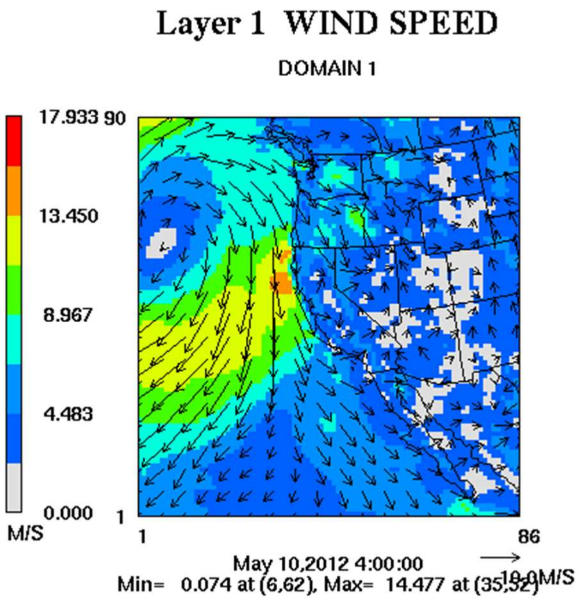


Fig. 6 The WRF model simulated wind speed and wind vector on domain 1.

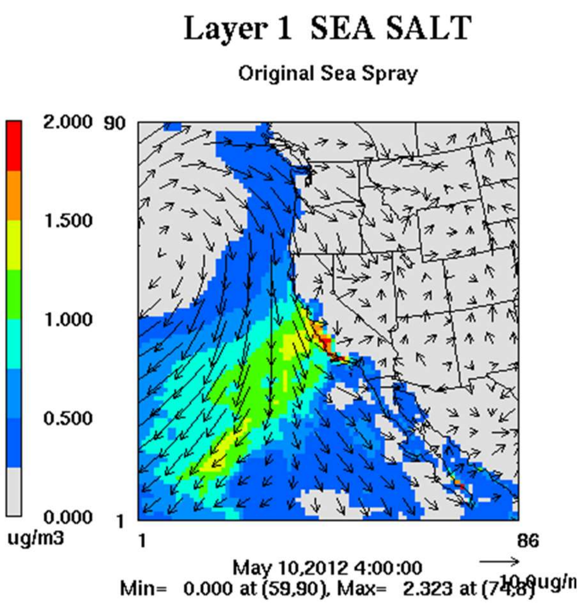


Fig. 7 The CMAQ simulated sea salt (with wind vector) on domain 1.

These results clearly show the under-prediction of sea salt by CMAQ. The magnitude of under-prediction ranges from a factor of 2 to a factor of 10. As a test, we increased the sea salt emission rate in the CMAQ model by a factor of 4 (Fig. 8). The patterns of sea salt, shown in Figs. 7 and 8, remain very similar (note an increase of 4 in the color scale in Fig. 8). The increase in sea salt emission by a factor of 4 actually increased the concentration of sea salt more than 4 times.

Figure 9 shows sea salt concentrations in domain 3 after sea salt emissions were increased by a factor of 4. We can clearly see the sea salt intrusion into the SFBA and the California Central Valley. Now, sea salt concentrations around San Francisco Bay are between 5 and 6 $\mu g/m^3$, much closer to the observations.

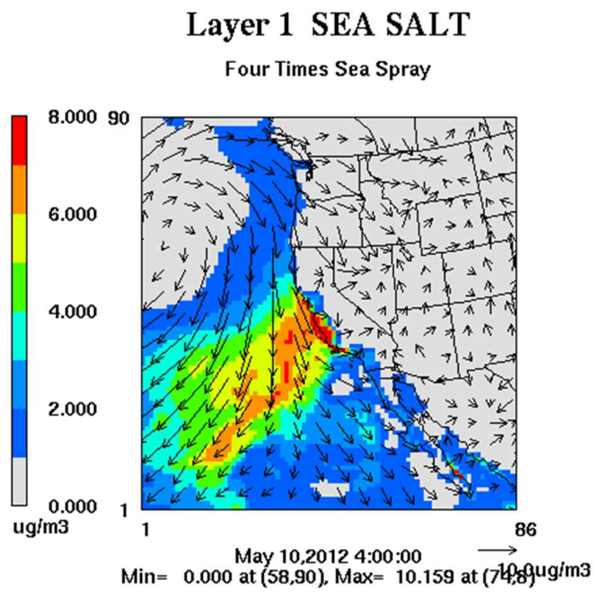


Fig. 8 The CMAQ simulated sea salt (with wind vector) on domain 1 using 4 times the sea salt emission rate.

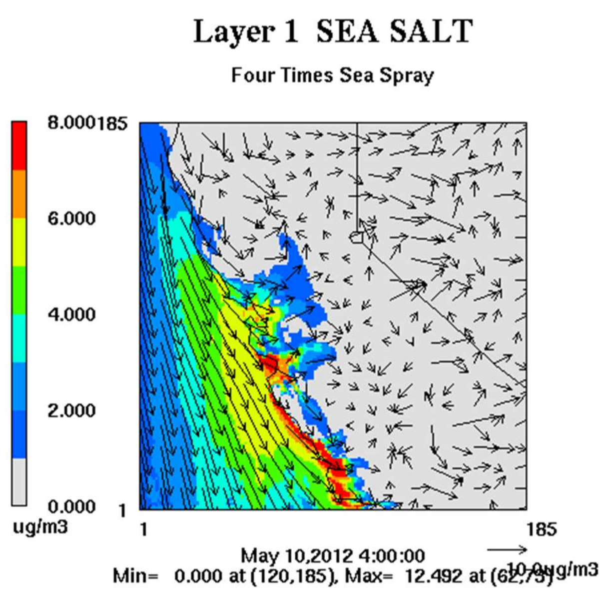


Fig. 9 The CMAQ simulated sea salt (with wind vector) on domain 3 using 4 times the sea salt emission rate.

Figure 10 shows a comparison of daily sea salt simulated with CMAQv5.0.2 to corresponding observations, both averaged over West Oakland, Vallejo and Livermore (observation data are only available for May 3, 9, and 15). Even with 4 times increased the sea salt emission rate, CMAQ version 5.0.2 still under-predicted sea salt by 30% on May 9, the day with high observed sea salt. On the two low sea salt days, it over-predicted sea salt on May 3 and under-predicted sea salt on May 15.

## 8. SEA SALT ENHANCEMENT IN CMAQv5.1

CMAQ version 5.1 was released after most of our experiments were finished. This version includes a revision that shifts some coarse mode sea salt to the accumulation mode. While experimenting with CMAQv5.1, we encountered a severe lateral boundary problem for PM. Large PM values, much larger than the values specified at the lateral boundary by MOZART data, periodically enter from the western boundary and greatly affect simulated PM2.5 in the SFBA. The model does give reasonable results using profile boundary conditions, which are relatively clean of PM.

Using profile boundary conditions, we proceeded to test the new version. Daily sea salt, simulated using CMAQv5.1 with the factor-of-4 increase in sea spray, is also shown in Fig. 10. Version 5.1 greatly improved sea salt predictions on all three days with observations. On May 9, the day with the largest observed sea salt, the simulation result is almost perfect.

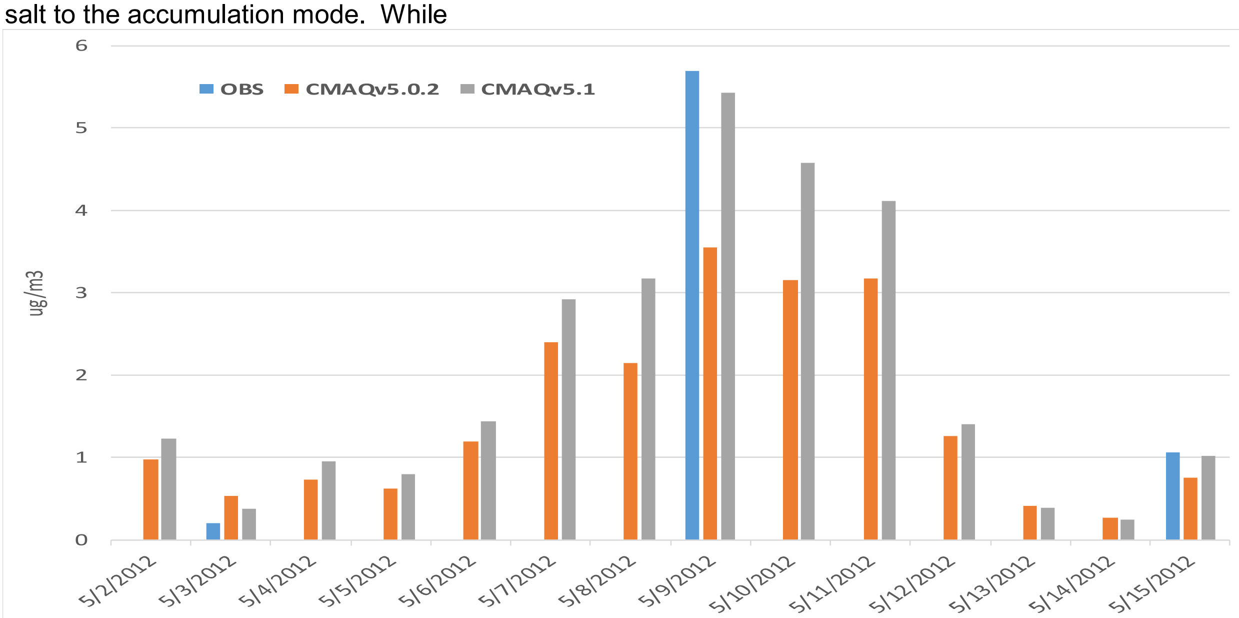


Fig. 10 Simulated sea salt with 4 times sea spray averaged over West Oakland, Vallejo and Livermore.

## 9. CONCLUDING REMARKS

We made year-round PM2.5 simulations for 2012 using CMAQv5.0.2 and found under-prediction of PM2.5 during the summer months. This under-prediction can be traced to the under-prediction of sea salt. An increase in sea salt emissions by a factor of 4 in the CMAQ model greatly improved the simulated sea salt. A simulation using CMAQv5.1, again with 4 times sea salt emissions, yielded simulated sea salt that almost matched observed sea salt in the SFBA.

We found problems with the lateral boundary treatment of PM species in the western and northern boundaries, i.e. the inflow boundaries. This problem created periodic unreasonably large inflows of PM into the domain and prevented us from using MOZART boundary conditions for the CMAQv5.1 runs.

For future work, we plan to collaborate with CMAQ model developers to refine sea salt emission rates and to resolve the problem in the lateral boundary treatment of PM species in CMAQv5.1.