J4.2 ASSESSMENT OF PM TRANSPORT PATTERNS USING ADVANCED CLUSTERING METHODS AND SIMULATIONS AROUND THE SAN FRANCISCO BAY AREA, CA

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1. INTRODUCTION

This study applied both cluster analysis and photochemical simulations to estimate representative fine particulate matter ($PM_{2.5}$) transport impacts. Clustering was first used to identify representative air flow patterns associated with potential pollutant transport into the San Francisco Bay Area (SFBA) of California. Then, photochemical simulation results were pooled across days assigned to the same transport pattern by the clustering. Pooling the data in this manner helped estimate representative transport impacts. The method was able to resolve and quantify patterns for $PM_{2.5}$ transport from two different areas that could be upwind of the SFBA, depending on the conditions.

2. STUDY DOMAIN

The SFBA (Figure 1) has recently been designated in nonattainment of the federal 24-hr $PM_{2.5}$ standard. SFBA 24-hr average $PM_{2.5}$ levels have exceeded the National Ambient Air Quality Standard (NAAQS) of 35 $\mu g/m^3$ on around 5-35 days per year since ambient measurements started in 1999. These exceedances occurred during the winter months. Stable boundary layers inhibited the dispersion of $PM_{2.5}$ and its precursors away from the surface. Exceedances involved significant impacts from both primary (directly emitted) as well as secondary $PM_{2.5}$ components. The secondary $PM_{2.5}$ was mostly ammonium nitrate and organic aerosol.

A previous study revealed that over 80% of the SFBA 24-hr $PM_{2.5}$ exceedances occurred under an air flow pattern for which winds entered the SFBA from across its eastern boundary (Beaver et al., 2009). The cartoon diagram in Figure 1 indicates the mechanism driving this flow pattern. It is termed the “R” flow pattern because it occurred when a strong aloft “ridge” of high pressure was positioned directly over Central California. Under these synoptic settings, the large-scale pressure gradient was weak, and low-level air flows developed locally. Persistent drainage (downslope) flows developed over the Central Valley rims due to nocturnal radiative cooling of the sloped terrain during cold clear winter nights. These flows converged toward the Central Valley floor, increasing the pressure within the Valley. A shallow easterly flow then emptied from the Central Valley through Carquinez Straight, the only major gap in the Central Valley rims. Easterly air flows extended through the SFBA and emptied over the Pacific Ocean. The R pattern was persistent and lasted for days to weeks when it occurred. SFBA $PM_{2.5}$ exceedances would usually occur after about 2-4 days of $PM_{2.5}$ buildup.

A polluted Central Valley air mass was likely transported into the SFBA by the R air flow pattern. The persistence of the R pattern provided the potential for considerable pollutant transport. Much of the transported $PM_{2.5}$ was believed to be ammonium nitrate. The Central Valley had much higher ammonium nitrate levels than the SFBA, especially deeper south into the San Joaquin Valley (SJV, Figure 2). Ammonium nitrate formed rapidly when available nitric acid reacted with intense ammonia emissions that were highly concentrated around the SJV dairying operations. Central Valley ammonium nitrate levels were regionally elevated because an aging air mass was typically trapped within the Central Valley for at least several days to weeks. Also, the cool inland winter temperatures inhibited evaporation of the formed ammonium nitrate particles. Ammonium nitrate levels were lower in the downwind SFBA (at San Jose) than for the upwind Central Valley. Ammonium nitrate levels were even lower further downwind at the remote coastal monitoring location at Point Reyes. These observations suggested that a plume of ammonium nitrate extended from the Central Valley, into the SFBA through Carquinez Strait, and over the Pacific Ocean under the shallow easterly air flow pattern.

3. METHODS

3.1 CLUSTER ANALYSIS

The previous cluster analysis of Beaver et al. (2010) focused on measurements from within the SFBA. In this current study, the same clustering technique was reapplied to an expanded spatial domain for the purpose of studying transport. Inputs to the clustering algorithm were from twelve SFBA weather stations included in the original clustering, plus an additional five weather stations from the northern SJV and around Sacramento. The purpose of this clustering was to determine if the Sacramento area and/or the SJV were consistently upwind of the SFBA during its $PM_{2.5}$ episodes.

The clustering algorithm was based on an Empirical Orthogonal Functions (EOF) decomposition of hourly 1-hr surface winds. The algorithm simultaneously low-pass filtered and clustered the input data to yield

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clusters defined by distinct EOF representations of the surface wind field. The low-pass filtering ensured the EOFs were estimated to reflect mostly synoptic (large-scale) influences on the surface winds. The large-scale conditions were resolved by compositing weather maps across the days assigned to each cluster. The algorithm identified real weather patterns reflecting fields coherent with the clustered wind field, including the large-scale pressure gradient.

The identified clusters were interpreted in two ways. First, the clusters were interpreted as static patterns. Data were pooled and averaged across the days assigned to each cluster. This described the average surface conditions associated with each generalized large-scale condition. The static patterns allowed inferences of recurring atmospheric processes responsible for pollutant buildup. Second, the clusters were interpreted as dynamic patterns. Sequences of daily cluster labels tracked the day-to-day evolution of the large-scale settings. Different types of $PM_{2.5}$ episodes were defined in terms of representative evolutions of the large-scale conditions.

3.2 PHOTOCHEMICAL SIMULATION

Photochemical $PM_{2.5}$ simulations for the Central California modeling domain (extent of Figure 1) were performed for the months of December and January of 2000-01 and 2006-07. The modeling domain had 4-km horizontal grid spacing. It included the SFBA, the SJV, and the Sacramento Valley (SV), as well as portions of the Pacific Ocean and the Sierra Nevada.

Meteorological fields were prepared using the Fifth-Generation National Center for Atmospheric Research (NCAR)/Pennsylvania State University Mesoscale Model (MM5). The model was run with 36-12-4 km two-way nested horizontal grids and with 30 vertical layers. The first layer was about 22 m deep. The model was re-initialized every 5 days. Winds were assimilated toward the analysis field.

Base case emissions inventories were prepared using the Sparse Matrix Operator Kernel Emissions (SMOKE) processor. Winter season emissions estimates were improved for many sources as part of the California Regional Particulate Air Quality Study (CRPAQS). Biogenic emissions were generated using the U.S. EPA beis2 program.

The gridded meteorological and emissions inputs were used to drive the Community Multiscale Air Quality (CMAQ) model for simulating base case $PM_{2.5}$ levels. Chemistry was simulated using the SAPRC99 mechanism and the AE3 aerosol module in conjunction with the Regional Acid Deposition Model (RADM) aqueous-phase chemistry model. The aloft layers from MM5 were collapsed to yield 16 vertical layers simulated by CMAQ. Model outputs were processed to yield 24-hr average (midnight to midnight, PST) levels for total, primary, and secondary $PM_{2.5}$. $PM_{2.5}$ components elemental carbon (EC), organic carbon (OC), nitrate, and sulfate were also extracted from the model output to perform model validation against speciated $PM_{2.5}$ measurements.

3.3 REPRESENTATIVE TRANSPORT IMPACTS

Two additional simulations were performed with emissions inventories modified relative to the base case. One inventory had anthropogenic emissions from the Sacramento area zeroed out, while the other inventory had anthropogenic emissions from the SJV zeroed out. These “transport runs” were implemented for the same four-month simulation period as for the base case. Differences in simulated $PM_{2.5}$ levels between either of these transport runs and the base case run indicated the amount of transported $PM_{2.5}$ from the Sacramento area or the SJV, respectively.

Representative transport impacts were estimated for each transport pattern detected by the clustering. For each transport pattern, impacts from both Sacramento area and the SJV were estimated separately using the respective CMAQ transport run outputs. For each transport pattern and upwind source region (Sacramento area or SJV), the respective model results were pooled across the days assigned to that transport pattern. Representative transport impacts were estimated for each model grid cell as the simple average of the pooled daily transport impacts.

4. RESULTS

4.1 CLUSTERING RESULTS

In total, 1001 winter (November-March) days from the years 1999-2007 were included in the transport cluster analysis. The clustering revealed six major winter weather patterns prevailing over the SFBA. Two of these weather patterns together accounted for most SFBA 24-hr $PM_{2.5}$ exceedances. Average surface flow patterns are shown in Figure 3. This pair of clusters was essentially the original R pattern split into two. The first pattern, named R-N, had northerly winds entering the Delta from the Sacramento area before passing into mostly the central and southern SFBA. The second pattern, named R-S, had southerly winds entering the Delta from the SJV before passing mostly into the eastern and northern SFBA. R-N and R-S accounted for around 60% and 20% of the SFBA 24-hr $PM_{2.5}$ exceedances, respectively. These transport patterns had distinct spatial distributions for $PM_{2.5}$, confirming their distinct source-receptor relationships. R-N had mostly uniform levels of $PM_{2.5}$ throughout the SFBA, with slightly higher $PM_{2.5}$ levels in the south SFBA (at San Jose). R-S had very high $PM_{2.5}$ levels in the eastern SFBA (at Concord and/or Livermore) and low to moderate $PM_{2.5}$ levels in the south SFBA.

R-N was a persistent weather pattern. It occurred when a ridge of aloft high pressure was positioned over Central California. Conditions were relatively calm and stable throughout Central California. Ammonium nitrate formed and accumulated in the Central Valley to high levels. Drainage flows over the Central Valley rims converged toward the Central Valley floor. Also, a shallow downvalley (northerly) flow developed along the SV major axis. This flow pattern had the potential to transport pollutants from the Sacramento area and the Delta into the SFBA. SFBA episodes under R-N could persist for up to weeks.

R-S was a transient weather pattern. It represented a transition from episodic R-N conditions into stormy and clean conditions. The aloft cyclonic counterclockwise motions of an approaching offshore low pressure center forced southerly winds through the complex Central Valley terrain. This flow pattern was deeper than for R-N, and conditions were becoming unstable and turbulent. But, the ammonium nitrate previously accumulated to high levels in the SJV was not dispersed immediately. The strong southerly R-S flows had the potential to transport ammonium nitrate northward into both the SFBA and the SV over the next 1-3 days. Clean conditions were achieved when the storm reached Central California and scoured the remaining pollutants from the sheltered valleys of the complex terrain.

Occurrences of R-N were not always followed by R-S. The R-N episodes could also terminate upon a direct transition into stormy conditions, without an intermediate occurrence of R-S. Pattern R-S only occurred immediately following R-N.

4.2 SIMULATION RESULTS

MM5 was tested using a number of available physics options. Operational evaluations were performed for the simulated fields generated using the various MM5 configurations. Simulated 1-hr surface winds, temperatures, and humidity were paired against observations archived at the National Center for Atmospheric Research (NCAR). The best performing physics options were selected to prepare meteorological inputs to CMAQ.

CMAQ was implemented using the MM5 and SMOKE outputs. Operational evaluation of the base case simulation $PM_{2.5}$ levels was performed using observations archived by the California Air Resources Board (ARB). Total 24-hr $PM_{2.5}$ levels were paired against simulated values from eleven monitors in the SFBA and three monitors near the Delta region. Speciated 24-hr $PM_{2.5}$ levels for EC and OC (both measured by the NIOSH method), nitrate, and sulfate were paired against simulated values from a single monitor in the south SFBA (at San Jose). For all evaluations, each observation was paired against the closest-matching simulated quantity within a 3×3 array of model grid cells surrounding the monitoring location. This pairing helped account for effects of the complex terrain— simulated $PM_{2.5}$ levels could vary considerably over relatively short distances. Simulated $PM_{2.5}$ levels correlated well against observations; however, simulated $PM_{2.5}$ levels during episodes were often underestimated relative to the observations. This effect appeared to have resulted mainly from the tendency of MM5 to overestimate the degree of vertical dispersion under strongly stable conditions. Horizontal air flows appeared to be reasonably well simulated.

Base case simulation results are shown in Figure 4 for a severe $PM_{2.5}$ episode that involved extreme levels of transport. Figure 4 (left) shows an occurrence of R-N on 5 January 2001, while Figure 4 (right) shows an occurrence of R-S on 7 January 2001. Transport impacts from the Sacramento area on 5 January (assigned to R-N) were calculated as the difference in $PM_{2.5}$ levels between the base case simulation and the transport run having the Sacramento area anthropogenic emissions zeroed out. Transport impacts from the Sacramento area on this day (not shown) were as high as 10 $\mu g/m^3$ in the eastern SFBA and were around 4 $\mu g/m^3$ at San Jose. Likewise, transport impacts from the SJV on 7 January (assigned to R-S) were as high as 45 g/m^3 in the eastern SFBA and were around 1 $\mu g/m^3$ at San Jose.

4.3 REPRESENTATIVE TRANSPORT IMPACTS RESULTS

Figure 5 shows representative transport impacts estimated using the method described in section 3.3. Transport impacts from the Sacramento area were averaged across 41 exceedance days occurring during the simulation period that were assigned to weather pattern R-N. Average transport impacts for these days were around 5-6 $\mu g/m^3$ in the eastern SFBA and around 2-4 $\mu g/m^3$ through the south SFBA, including San Jose. This transported $PM_{2.5}$ was about half primary and half secondary. Transport impacts from the SJV were averaged across 5 exceedance days occurring during the simulation period that were assigned to weather pattern R-S. Average transport impacts for these days were around 15 $\mu g/m^3$ in the eastern SFBA and around 6-9 $\mu g/m^3$ through the northern SFBA. This transported $PM_{2.5}$ was about two-thirds secondary and one-third primary. The San Jose location was on average not strongly impacted by transport from the SJV under the R-S air flow pattern.

5. DISCUSSION

The performance of MM5-CMAQ to reproduce the transport associated with the R-N and R-S flow patterns was verified for an extreme SFBA $PM_{2.5}$ episode terminating on 7 January 2001. On 5 January, R-N had persisted for 11 days, all of which were 24-hr $PM_{2.5}$ exceedances in the SFBA. Figure 4 (left) shows the simulated 24-hr $PM_{2.5}$ levels and 24-hr surface layer wind field for this day. The simulation reproduced several important aspects of the episode that were consistent with the R-N transport pattern. First, transport of $PM_{2.5}$ was evident from the southern SV and through the SFBA, resulting in a plume of $PM_{2.5}$ extending from the SFBA and over the Pacific Ocean. Second, maximum SFBA $PM_{2.5}$ level was simulated in the south SFBA (around San Jose). Third, SJV conditions were stagnating, and ammonium nitrate was accumulated to high levels. As the storm approached, R-S occurred on 6-7 January. Winds shifted to southerly, and any accumulated pollutants were transported northward. During the 2-day occurrence of R-S, SFBA $PM_{2.5}$ levels increased in the eastern and northern locations but decreased in the central and southern locations. Model results for 7 January are shown in Figure 4 (right). The simulation accurately reproduced the transport of the polluted SJV air mass through the eastern and northern SFBA. The highest SFBA $PM_{2.5}$ levels both occurred and were simulated in the eastern SFBA (around Concord). Observed and simulated $PM_{2.5}$ levels in the central and southern SFBA were relatively low.

Analysis of the above extreme transport event helped validate the simulation as being mechanistically consistent with the conceptual model derived from the clustering. Similar model performance was obtained for other transport events identified by the clustering; however, because the level of transport was lower, it was more difficult to verify against the observations. Simulation of the extreme transport event also demonstrated that exceedances could occur in the SFBA from transported pollutants alone, without any SFBA emissions. These results were, however, not representative because of the extreme nature of this single episode.

The representative transport impacts shown in Figure 5 were estimated by pooling the model results across a moderate number of exceedance days identified by the clustering to have exhibited similar transport characteristics. Pooling the model results as such helped to down weight the impacts of extreme transport events, such as the SFBA $PM_{2.5}$ exceedance occurring on 7 January 2001. Transport impact from the SJV on this extreme day was around five times greater than the average impact shown in Figure 5. This finding is important because this day was part of the CRPAQS field campaign and will likely be modeled extensively by other researchers. Future $PM_{2.5}$ transport research should address representative, and not extreme, transport events.

6. CONCLUSIONS

The SFBA appeared to be significantly impacted by $PM_{2.5}$ transported from both the Sacramento area and the SJV. The relative impacts of these upwind source areas on SFBA $PM_{2.5}$ levels depended on the conditions. A persistent episodic weather pattern was associated mostly with transport from the Sacramento area. A transient episodic weather pattern was associated mostly with transport from the SJV. Transport from the Sacramento area accounted for around four times as many 24-hr $PM_{2.5}$ exceedance days in the SFBA as compared to transport from the SJV; however, transport impacts from the SJV were usually larger in magnitude.

There were differences in the spatial distribution and composition of the $PM_{2.5}$ transported from the two upwind regions. $PM_{2.5}$ transported from the Sacramento area was simulated as around half primary and half secondary. $PM_{2.5}$ transported from the SJV was simulated as mostly secondary $PM_{2.5}$, especially ammonium nitrate. This finding suggested that SJV ammonia emissions from concentrated dairying operations significantly impacted SFBA winter air quality.

REFERENCES

Beaver, S., Palazoglu, A., Singh, A., Soong S.T., and Tanrikulu, S., 2010: Identification of winter weather patterns impacting 24-hour average fine particulate matter levels. *Atmos. Environ.*, in press. DOI 10.1016/j.atmosenv.2010.02.001.

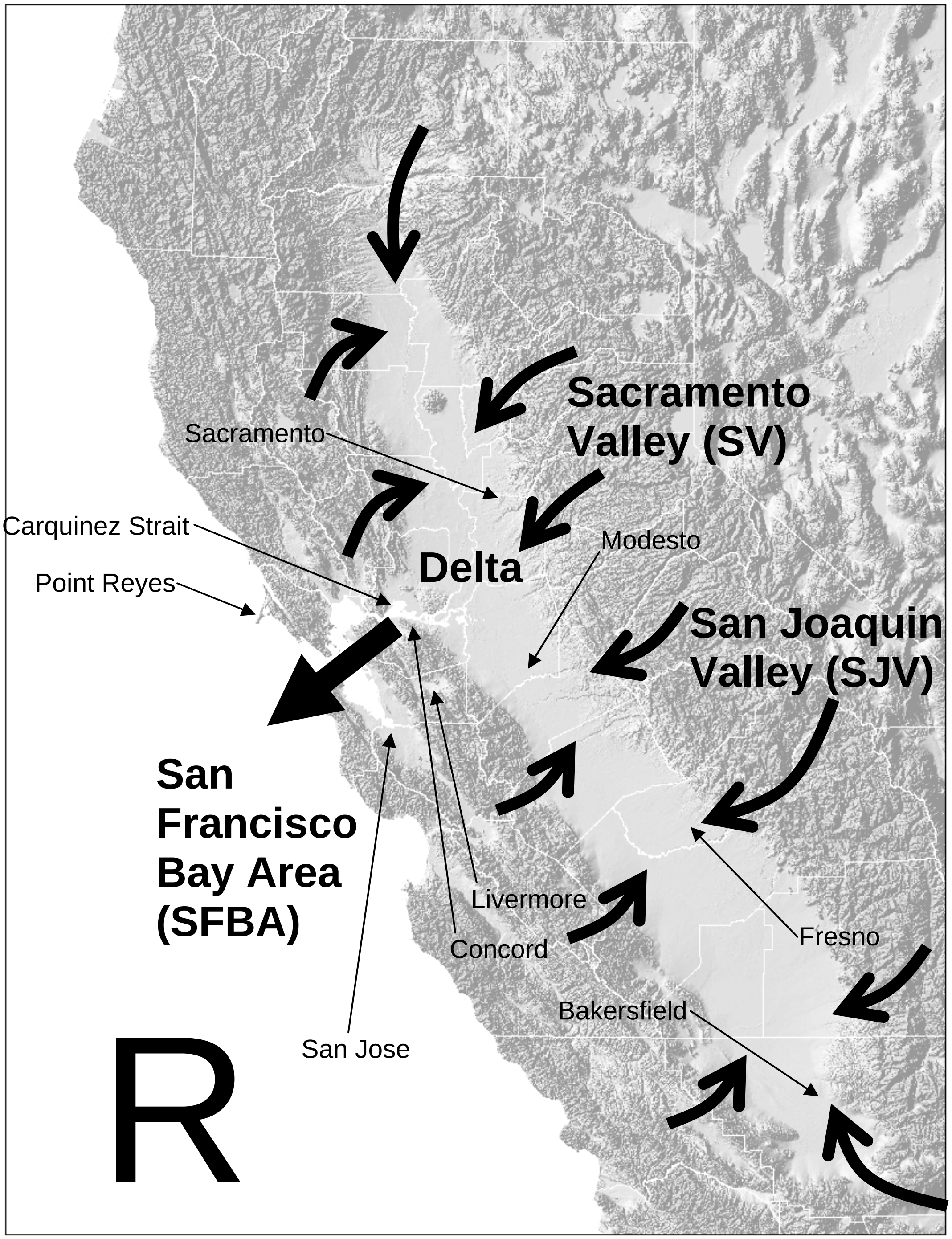

Figure 1. Central California photochemical modeling domain. Central Valley comprises SV to the north and SJV to the south, joined at the Delta region. Locations described in the text are denoted. Cartoon indicates R air flow pattern associated with most SFBA 24-hr $PM_{2.5}$ exceedance days. Curved arrows over Central Valley slopes indicate downslope flows. Block arrow indicates Central Valley exit flow through Carquinez Strait.

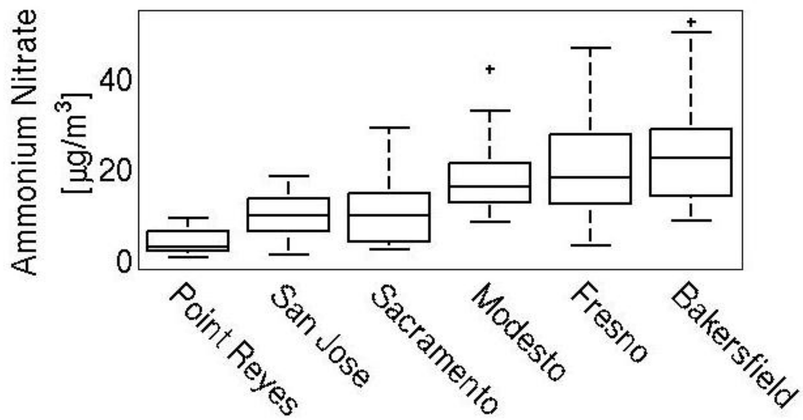

Figure 2: Ammonium nitrate levels during R air flow pattern at a background location (Point Reyes), south SFBA (San Jose), and Central Valley (see Figure 1). Stations are sorted left to right from a coastal location to further inland. Horizontal lines on boxes indicate lower quartile, median, and upper quartile. Whiskers extend 1.5 times the interquartile range (box length). Outliers are indicated using plus signs (+).

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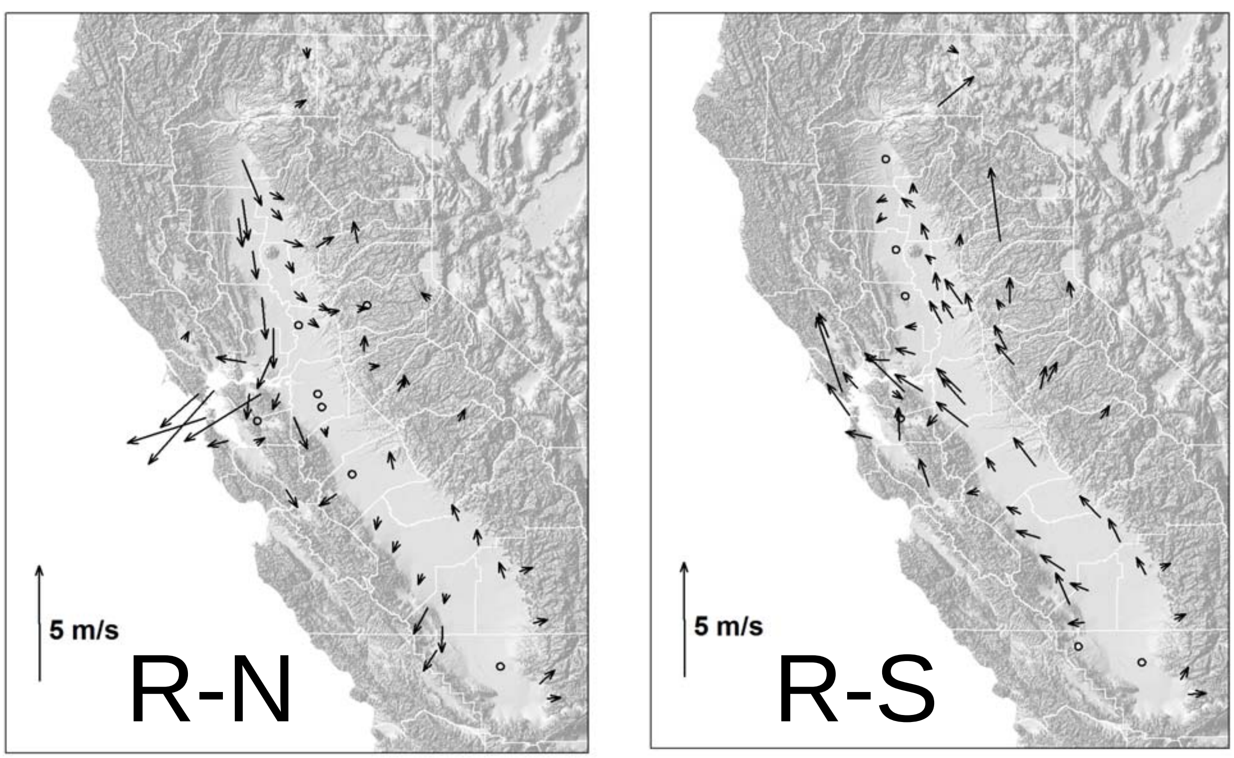

Figure 3: Pair of episodic weather patterns with potential for transport into the SFBA: R-N (left) and R-S (right). Mean surface 1-hr air flows are shown at 0900 PST for SFBA and Central Valley weather stations.

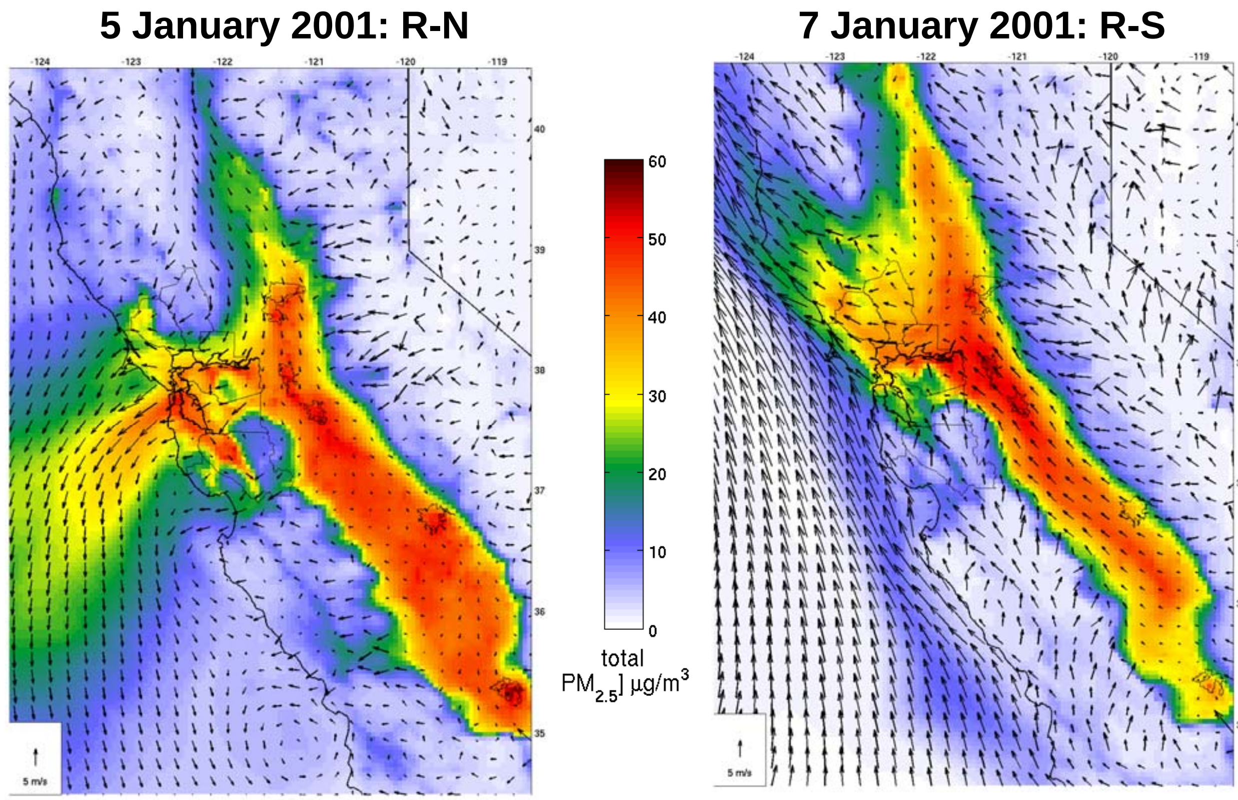

Figure 4: Base case simulation results for an extreme transport event. Simulated 24-hr surface winds and 24-hr total $PM_{2.5}$ levels are shown for two days from 2000-01 winter. R-N occurred on 5 January, and R-S occurred on 7 January.

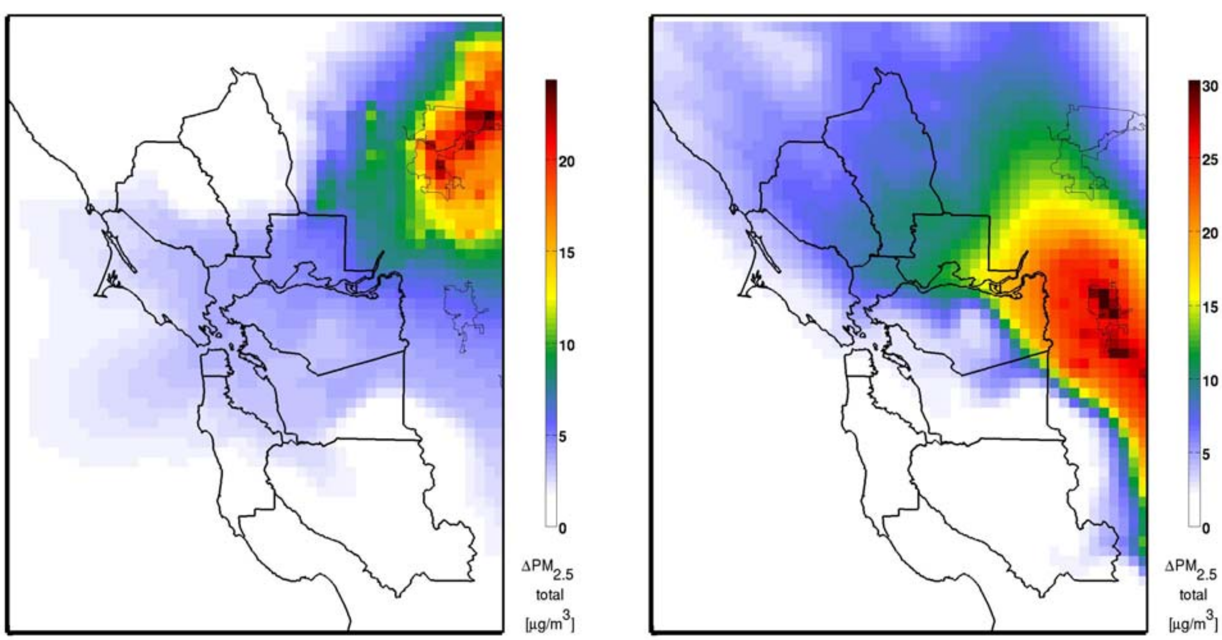

Figure 5: Representative transport impacts on SFBA. Left panel shows impact of Sacramento area emissions, averaged across 41 SFBA $PM_{2.5}$ exceedance days assigned to R-N. Right panel shows impact of SJV emissions, averaged across 5 SFBA $PM_{2.5}$ exceedance days assigned to R-S.