EVALUATING METEOROLOGICAL INPUTS TO AIR QUALITY MODELS WITH INERT TRACER SIMULATIONS

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1. INTRODUCTION

Evaluations of meteorological models have often focused on how well model predictions and observation of specific variables match. In past summertime studies, efforts have been made to evaluate a model's ability to represent mixing-layer depths; the vertical distributions of winds, temperature, and humidity; up-slope and down-slope flows; marine-layer intrusions; and large-scale eddies. Less work has been performed on the evaluation of wintertime phenomena, particularly under extended stagnation conditions when horizontal transport becomes small and vertical transport and mixing processes are very important. From an air quality perspective, we know that correctly modeling all phenomena that affect transport and diffusion is more important than correctly modeling individual variables.

The abilities of two meteorological models to maintain mass within California's Central Valley (CV) (see **Figure 1**) were assessed using inert tracer simulations of winter particulate matter (PM) less than 2.5 µm ($PM_{2.5}$) episodes that occurred in the San Joaquin Valley (SJV) during the California Regional $PM_{10}/PM_{2.5}$ Air Quality Study (CRPAQS) field program. Tagged tracer simulations were also performed to investigate each model's representation of transport within and between air basins.

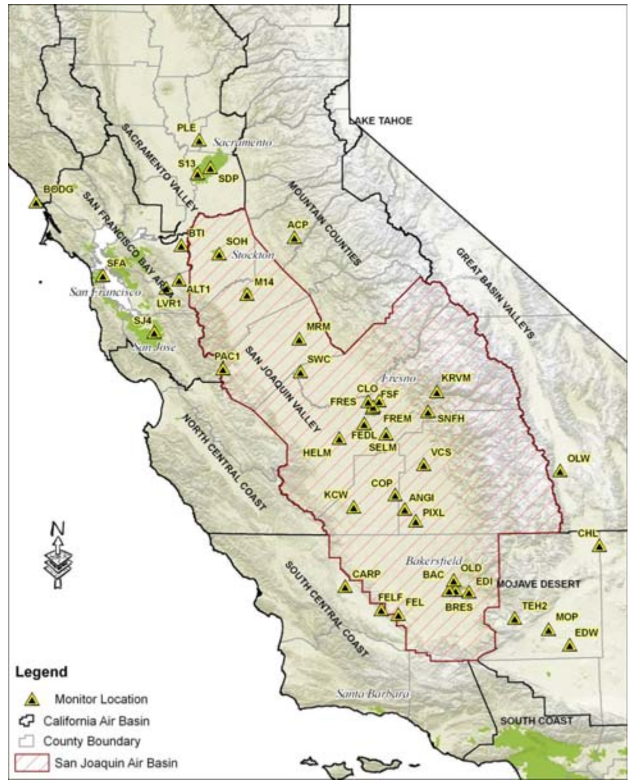

Fig 1. The Central Valley (CV) of California includes the Sacramento Valley (SV) and San Joaquin Valley (SJV).

2. APPROACH

A series of simulations were performed with the Comprehensive Air Quality Model with Extensions (CAMx) (ENVIRON International Corporation, 2004) to assess the role of transport and diffusion during wintertime SJV pollution episodes, and to assess the ability of two meteorological models, the Pennsylvania State University/National Center for Atmospheric Research Mesoscale Model, Version 5 (MM5) (Grell et al., 1994) and the CALMET model (Scire et al., 2000), to reproduce important meteorological phenomena that contributed to these episodes. We used CAMx for its ability to predict the three-dimensional evolution of inert tracers using meteorology from MM5 and CALMET.

2.1 Inert Tracer Conservation

To perform a test of tracer gas conservation, we processed the MM5 output with the MM5CAMX programs and the CALMET output with the CMETCAMX program, to develop CAMx-ready meteorological inputs. The CAMx domain was uniformly initialized with a 1,000 ppb concentration of an inert tracer gas. Advection and turbulent diffusion were allowed to act on the tracer field, but there were no tracer sources or sinks within the domain. To allow tracer mass to exit the domain but not enter, tracer concentrations at the top and lateral boundaries of the model were set to negligibly small values.

Four simulations were performed. CAMx was executed with MM5 meteorological inputs and with CALMET meteorological inputs for two CRPAQS

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episodes: December 25-30, 2000, and January 3-8, 2001. The same horizontal grid consisting of 185 x 185, 4-km cells on a Lambert Conformal projection was used for all simulations. When the meteorological fields were prepared for CAMx, the CAMx vertical grid structure was determined by the vertical grid structure of the model that provided the meteorological fields to prevent vertical interpolation errors when the meteorological fields were mapped to the CAMx grid. The vertical grid structures of the two meteorological models differed substantially. MM5 used a 30-layer grid that spanned beyond the tropopause, while CALMET used a 20-layer grid with a domain top at 2,750 m.

Vertical diffusivity fields are needed for input to CAMx. Since vertical diffusivity is not predicted by the meteorological models, it must be derived based on wind, temperature, and/or other planetary boundary layer parameters. The method of O'Brien (1970) was used to derive vertical diffusivity values from both MM5 and CALMET output.

2.2 Tagged Tracers

An additional series of CAMx experiments were performed to evaluate transport within the SJV during the CRPAQS $PM_{2.5}$ episodes. Unique inert tracers were assigned to the following urban areas: Bakersfield, Visalia, Fresno, Modesto/Stockton, Sacramento, and the San Francisco Bay Area. An additional tracer was assigned to all other (primarily rural) grid cells. Emitted tracers were thus "tagged" with their location of origin and could be tracked as they were advected and diffused in the CAMx domain.

Urban boundaries were objectively drawn to encapsulate regions with the largest emissions. Tracer emission rates were scaled to weekday NO_x emissions in a gridded regional inventory. NO_x was chosen because NO_x concentrations are expected to scale with primary PM emissions and secondary PM production.

The CAMx grid was initialized with zero concentrations for all seven tracers. The various tracers were continuously emitted from ground-level sources into the first model layer. Advection and turbulent diffusion then acted on these emissions. Because the tracers are inert and there are no sinks, the tracers from different regions could be tracked for further analysis. As in the mass conservation tests, tracer mass may exit but not enter the modeling domain.

Five simulations were performed. CAMx was executed twice for each study episode, once with MM5 meteorological inputs and once with CALMET meteorological inputs. The study episodes coincide with the same episodes modeled in the inert tracer conservation simulation. A fifth simulation, based on MM5 meteorology, was performed for December 23, 2000, to January 10, 2001, to investigate transport over a longer period.

3. RESULTS

3.1 Inert Tracer Conservation

An evaluation of the tracer evolution in these simulations shed light on the ability of the meteorological models to maintain mass within the SJV. For both the December 2000 and January 2001 simulations, CAMx simulations with MM5 meteorology maintained substantially more tracer mass within the SJV than simulations with CALMET meteorology.

December 2000

During the first 24 hours, air devoid of tracer mass was advected into the domain, predominantly from the east. This advection, combined with the strong vertical mixing over the mountains of Nevada and California, removed tracer mass from much of the domain within the first 24 hours. In both episodes, most of the remaining mass at the surface after 24 hours was in the CV. Peak valley tracer concentrations after 24 hours were 1,000 ppb in the MM5-based simulation, and close to 1,000 ppb in the CALMET-based simulation. However, spatial plots of surface tracer mass already indicated a mass loss in the CALMET simulation relative to the MM5-based simulation. Surface concentrations in the MM5-based simulation were over 900 ppb throughout the CV; but in the CALMET-based simulations, some portions of the CV were already below 700 ppb, and only a few small regions remained with concentrations over 800 ppb.

During the second 24 hours, substantial CV tracer mass was lost in the CALMET-based simulation. By the end of day 2, peak surface tracer concentrations within the CV in the CALMET-based simulation dropped to about 500 ppb, half the initial concentration. Tracer mass in the CV was also lost in the MM5-based simulation but at a much slower rate; the peak valley concentration was 860 ppb (85% of the initial concentration) by the end of day 2. A solid region of tracer concentrations over 600 ppb filled much of the CV in the MM5-based simulation; but in the CALMET-based simulation, most of the remaining mass was confined to the narrow strip in the western and central portions of the CV. The 100 ppb contour no longer filled the entire CV, and most of the tracer had been completely dispersed in the northern SV.

Concentrations continued to decline during day 3. The midday, ground-level tracer concentrations for the CALMET-based simulation are shown in **Figure 2** and for the MM5-based simulation in **Figure 3**. At the end of day 3, most of the concentrations in the CV had dropped below 100 ppb in the CALMET-based simulation, while concentrations in much of the CV from Sacramento southward were above 400 ppb in the MM5-based simulation.

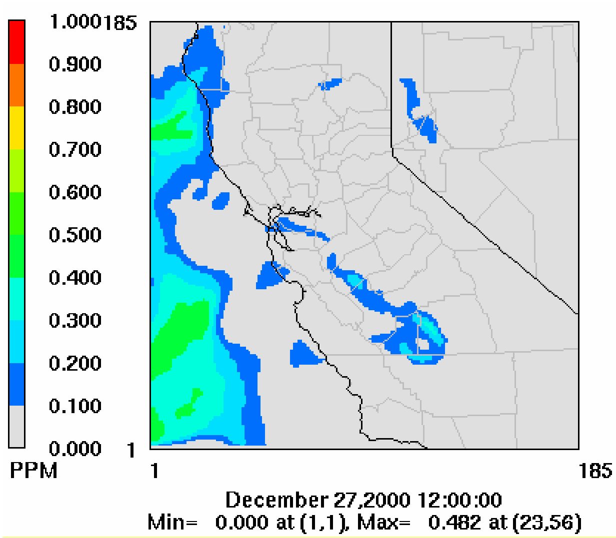

Fig 2. CAMx predicted tracer concentrations after 60 hours using CALMET meteorology.

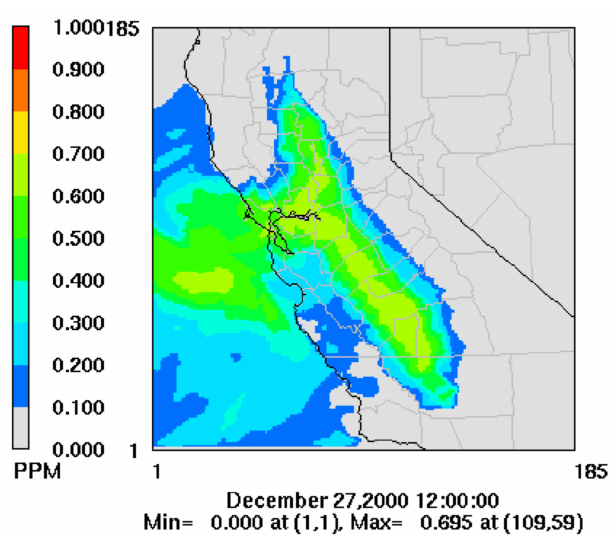

Fig 3. CAMx predicted tracer concentrations after 60 hours using MM5 meteorology.

In the MM5-based simulation, peak CV tracer concentrations remained above 500 ppb (50% of the initial concentration) through hour 80 (3.3 days). Even by the end of the simulation, peak CV concentrations remained above 200 ppb. By hour 72, no substantial area of tracer concentrations above 100 ppb remained in the CV in the CALMET-based simulation. The MM5-based simulation retained a large area of concentrations greater than 100 ppb in the CV throughout the entire simulation. Residence time for tracer mass within the CV aloft was also longer in the MM5-based simulation than in the CALMET-based simulation.

January 2001

Similar results were observed in the January 2001 inert tracer simulations; the MM5-based simulation was more successful at retaining mass within the SJV than the CALMET-based simulation. Both January simulations suggest increased stagnation in the SJV compared to that suggested by the December simulations. Peak SV surface tracer concentrations remained above 500 ppb through hour 104 in the MM5 case (compared to hour 80 in December), and through hour 72 in the CALMET-based simulation (compared to hour 70 in the December episode). This trend is consistent with PM observations that indicated higher peak concentrations during the January 3-8 episode than the December 25-30 episode.

Possible Factors for Mass Losses

An analysis of the mass balance in CAMx indicated that significant mass in the CALMET-based simulations was lost through the top boundary. This loss may be a result of the top boundary being only 2.75 km above ground level. In the CALMET-based simulations, more tracer mass (relative to MM5-based simulations) was also lost through the coastal mountains along the western side of the SJV, particularly through Cottonwood Pass in the southern SJV and through Pacheco Pass in the central SJV.

Enhanced convergence in the CALMET wind fields appeared to occur in some regions, particularly near mountains. In those regions, tracer mass in the CALMET-based simulations was lofted from the surface and transported out of the model domain either through the top or lateral boundaries. In addition to mass loss through the western coastal mountains, tracer mass exited aloft (1-km agl) through the southern end of the SJV and through Donner Pass in the Sierra Nevada Mountains.

3.2 Tagged Tracers

Local tracer emissions dominated the total tracer concentrations, though a significant fraction of the total tracer concentrations at urban sites came from rural areas. For example, at Visalia the CALMET-based simulation for the December episode showed, on average, that 79% of the inert tracer material came from local sources with the remaining 21% mostly from non-urban (other) sources as shown in **Figure 4**.

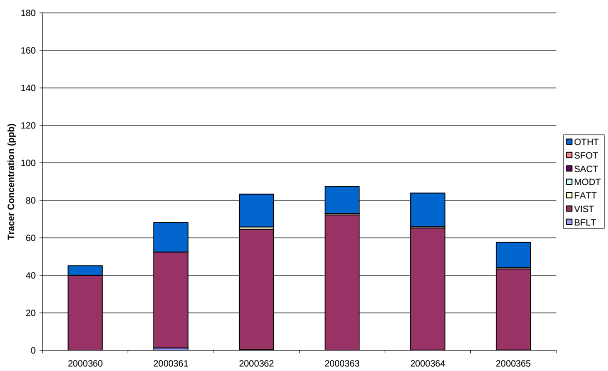

Fig 4. Predicted contributions of inert tracers at Visalia for December 26-31, 2000, based on CALMET meteorology.

The MM5-based simulation results (**Figure 5**) showed only 57% of the inert tracer was local with the remaining contributions associated with rural, Fresno, Stockton/Modesto, and Sacramento emissions.

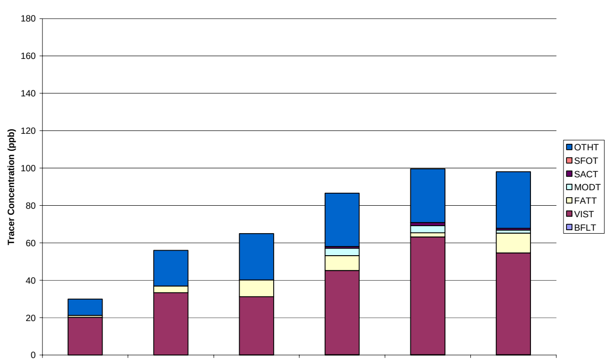

Fig 5. Predicted contributions of inert tracers at Visalia for December 26-31, 2000, based on MM5 meteorology.

The relative contribution of rural tracers at urban sites was less in CALMET-based simulations than in MM5-based simulations. Also, the relative contribution of non-local tracers (that is, tracers not emitted from the location selected for analysis) was larger in MM5- than CALMET-based simulations. For example, at Visalia in the December episode, the MM5 simulation predicted 3-9 ppb of tracer from Fresno on some days, whereas in the CALMET-based simulation, almost no Fresno tracer was present at Visalia. For the January episode, the total tracer at Stockton contained some contribution from Sacramento in the MM5 simulation, but little or no Sacramento contribution in the MM5 case.

These results imply that the MM5 wind field allows more transport within the SJV compared to the CALMET wind field. This result was unexpected considering that MM5 was found to consistently underpredict wind speeds in the SJV. Increased vertical mixing due to enhanced vertical diffusion or enhanced surface convergence could also contribute to the perceived lack of horizontal transport in the CALMET simulations.

As expected, rural sites, such as Angiola, had lower total tracer concentrations than urban sites, and the total tracer concentrations at rural sites were larger in the MM5-based simulation than in the CALMET-based simulation. The difference was large at Angiola (50-60%) but much smaller at Elk Grove. All simulations produced peak tracer concentrations of at least 20 ppb (20 ppb for the CALMET-based simulation and 38 ppb for the MM5-based simulation) at Angiola. This is important because the PM episode during CRPAQS was widespread, and rural emissions sources, though weaker than urban sources, are distributed throughout the SJV. Collectively, these rural emissions could add significant amounts of precursor pollutants to the atmosphere.

At Fresno, Bakersfield, and Angiola during the December episode, the MM5-based simulation predicted an upward trend in daily average total tracer concentrations. This trend continued through the entire simulation, except at Fresno where the tracer concentrations dropped slightly on the last day. These upward trends coincided with the observed upward trend in daily average $PM_{2.5}$ during the episode at all three sites. The CALMET-based simulation produced large tracer concentrations quickly at Fresno, possibly due to reduced transport and the resultant enhanced effect of local emissions; thus the upward trend was not maintained through the simulation. At Bakersfield and Angiola, the CALMET-based simulation predicted a trend of increasing concentrations through the third or fourth day. On the fifth day (sixth day for Angiola), the total tracer concentrations dropped in the CALMET-based simulation, while they continued to increase in the MM5-based simulation. At many of the analysis sites, the upward trend continued in the MM5-based simulation, but in the CALMET-based simulation, the upward trend either flattened or dropped off on the last day. This discrepancy may be an artifact of the inability to retain mass in the SJV with the CALMET-based simulations.

In the SV, the MM5-based simulation produced a sharp decrease in concentrations on the last day of the December episode, whereas the drop in tracer concentrations was less severe for the CALMET-based simulation. Neither simulation reproduced the observed PM trend in Sacramento, where peak PM was observed on the last two days. During the inert tracer experiment, it was noted that both simulations had more difficulty preserving mass in the SV than in the SJV.

4. SUMMARY AND CONCLUSIONS

The abilities of two meteorological models to maintain simulated mass within California's Central Valley were assessed using inert tracer simulations of winter $PM_{2.5}$ episodes that occurred in the SJV during the CRPAQS field study. Tagged tracer simulations were performed to investigate each model's representation of transport within and between air basins.

CAMx simulations with MM5 meteorology maintained substantially more tracer mass within the modeling domain than simulations with CALMET meteorology. CALMET-based simulations lost mass through the model's lateral and top boundaries, which may have been a result of divergence introduced by using inappropriate observations.

Based on the tagged tracer simulations, it appears that MM5 wind fields allowed more transport within the SJV compared to the CALMET wind fields. This is a potentially important result because the CALMET model has been used in previous studies (MacDonald et al., 2006) to conclude that minimal transport occurs within the SJV during wintertime stagnation conditions.

The use of inert tracer simulations was found to be a useful technique in comparing meteorological models and diagnosing potential problems in the modeling systems. Although this technique was used to evaluate two very different meteorological models, it should be useful in comparing different options for the same model.

5. ACKNOWLEDGEMENTS

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