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Ozone Formation in California's San Joaquin Valley: A Critical Assessment of Modeling and Data Needs

Betty K. Pun [a], Jean-François Louis [a], Prasad Pai [a], Christian Seigneur [a], Sam Altshuler [b] & Guido Franco [c]

[a] Atmospheric and Environmental Research, Inc., San Ramon, California, USA

[b] Pacific Gas and Electric Company, San Ramon, California, USA

[c] California Energy Commission, Sacramento, California, USA

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Ozone Formation in California's San Joaquin Valley: A Critical Assessment of Modeling and Data Needs

Betty K. Pun, Jean-François Louis, Prasad Pai, and Christian Seigneur
Atmospheric and Environmental Research, Inc., San Ramon, California

Sam Altshuler
Pacific Gas and Electric Company, San Ramon, California

Guido Franco
California Energy Commission, Sacramento, California

ABSTRACT

Data from the 1990 San Joaquin Valley Air Quality Study/ Atmospheric Utility Signatures, Predictions, and Experiments (SJVAQS/AUSPEX) field program in California's San Joaquin Valley (SJV) suggest that both urban and rural areas would have difficulty meeting an 8-hr average O_3 standard of 80 ppb. A conceptual model of O_3 formation and accumulation in the SJV is formulated based on the chemical, meteorological, and tracer data from SJVAQS/ AUSPEX. Two major phenomena appear to lead to high O_3 concentrations in the SJV: (1) transport of O_3 and precursors from upwind areas (primarily the San Francisco Bay Area, but also the Sacramento Valley) into the SJV, affecting the northern part of the valley, and (2) emissions of precursors, mixing, transport (including long-range transport), and atmospheric reactions within the SJV responsible for regional and urban-scale (e.g., downwind of Fresno and Bakersfield) distributions of O_3. Using this conceptual model, we then conduct a critical evaluation of the meteorological model and air quality model. Areas of model improvements and data needed to understand and properly simulate O_3 formation in the SJV are highlighted.

IMPLICATIONS

The development of State Implementation Plans to address the O_3 air quality standard will require meteorological and air quality models that provide accurate representations of the relevant atmospheric processes over regional scales. The California SJV is an appropriate test bed for evaluating state-of-the-science models, because of its variety of chemical and meteorological regimes and the availability of data to execute and test models. A conceptual model of O_3 formation in the SJV was developed and used to critically assess the suitability of meteorological and air quality models. Specific recommendations are provided to improve existing models, thereby increasing the level of confidence in the use of model predictions of O_3 and precursors to develop cost-effective emission control strategies.

INTRODUCTION

Summertime O_3 air pollution is a serious problem in California's San Joaquin Valley (SJV). The 1990 San Joaquin Valley Air Quality Study (SJVAQS) and the Atmospheric Utility Signatures, Predictions, and Experiments (AUSPEX) were two components of a comprehensive study to address this issue.[1] The comprehensive study involved (1) a large-scale air quality measurement program, (2) analyses of the causes of poor O_3 air quality, and (3) the development and application of a regional-scale air quality modeling system (SJVAQS/AUSPEX Regional Model Adaptation Project, or SARMAP). The field program was conducted during an eight-week period from July 9, 1990, to August 24, 1990. Fourteen intensive days were selected, which corresponded to high O_3 episodes, for detailed measurements. Figure 1 depicts the SJVAQS/AUSPEX domain.[1]

Time series of the daily maximum 1-hr and 8-hr average O_3 concentrations are shown in Figures 2 and 3, respectively.[2] At urban sites, the 8-hr average concentrations can be 20 to 30 ppb lower than the 1-hr maximum when O_3 concentrations are above 100 ppb (e.g., in Fresno). On the other hand, at rural sites such as Sequoia National Park, the daily maximum 8-hr concentrations of O_3 tend to be similar (< 10 ppb difference) to the daily 1-hr maximum concentrations. As a result, while urban areas exceed the 1-hr average National Ambient Air Quality Standard (NAAQS) of 120 ppb, both urban and rural areas may exceed an 8-hr average NAAQS of 80 ppb.

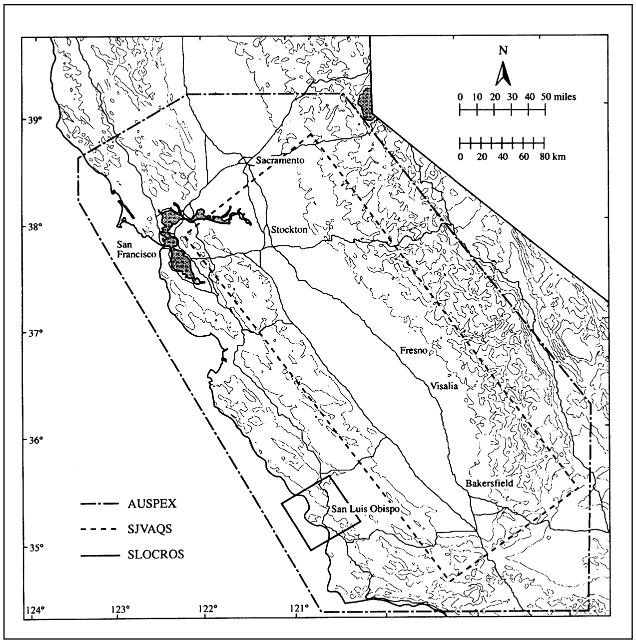

Figure 1. The study domain of SJVAQS/AUSPEX (reprinted with permission from Ranzieri and Thuillier,[1] copyright CRC Press, Boca Raton, FL, p 25).

Our objectives are to (1) construct an integrated analysis of O_3 formation in the SJV and (2) use it to critically assess whether existing meteorological and air quality models can accurately describe the major relevant processes. First, we build upon previous data analyses and develop a conceptual model of summertime O_3 formation in the SJV, which combines our knowledge of chemical processes with that of transport processes. Previous investigators have analyzed the ambient chemistry and aerosol data,[3] and the meteorological and tracer data[4-6] of the SJVAQS/AUSPEX program. However, none of those analyses provided an integrated analysis of the chemistry and transport processes leading to O_3 formation in the SJV.

Second, we assess the ability of current mathematical models of meteorology and air quality to provide an accurate description of the major causes for O_3 formation identified in the conceptual model. As discussed below, the SJV presents a wide variety of conditions for atmospheric chemistry and meteorology. Therefore, our assessment of model capabilities should find applications to other areas besides the SJV. In terms of model evaluation, our approach differs from the more typical approach that involves comparing model predictions with observations. We believe that such comparisons provide only limited insights in the model weaknesses unless the observational database is comprehensive enough to allow a detailed diagnostic evaluation of the models. Thus, our evaluation of the model formulation with respect to the conceptual model is complementary to the standard model performance evaluation approach.

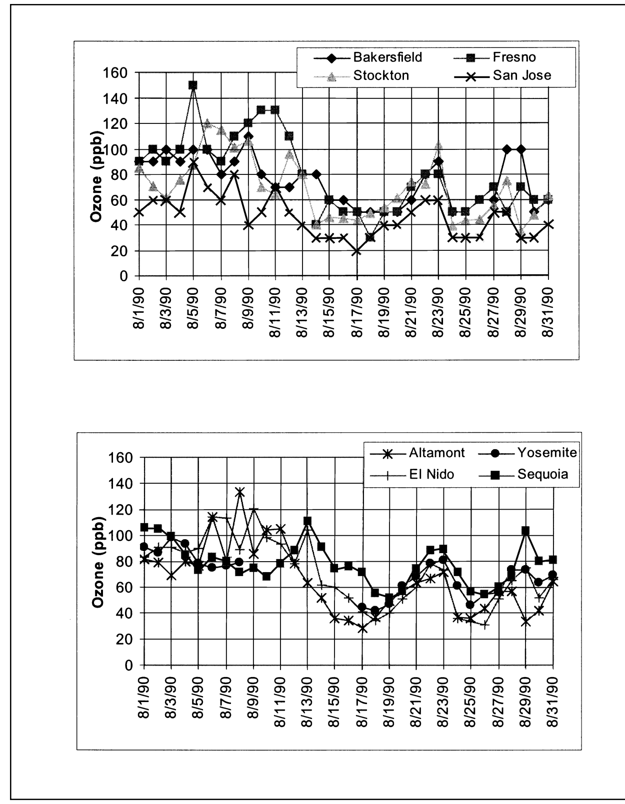

Figure 2. Daily maximum 1-hr average ozone concentrations at selected sites.[2]

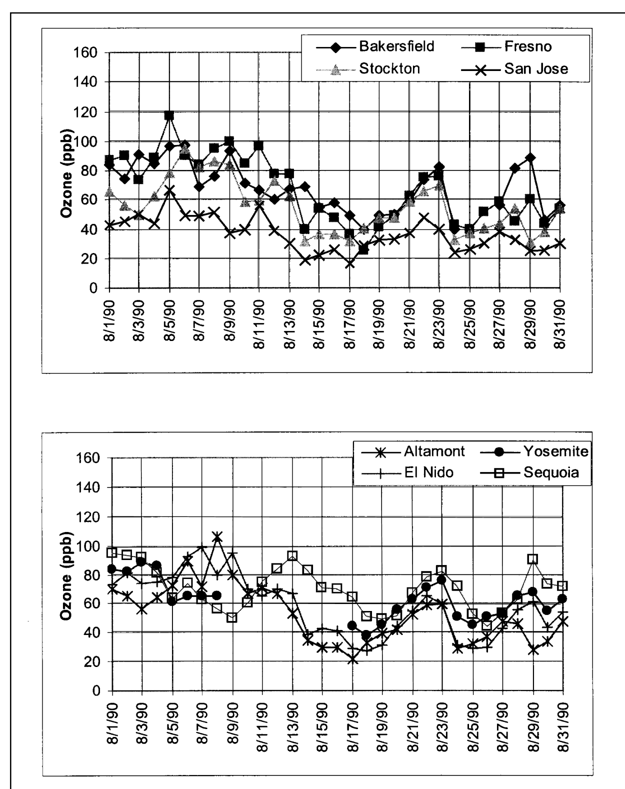

Figure 3. Daily maximum 8-hr average ozone concentrations at selected sites.[2]

Following these analyses, we highlight areas for additional data collection needed for rigorous model evaluation, including diagnostic model evaluation, and areas of improvements to existing mathematical models. Additional model evaluation and improvement activities allow us to gain confidence that the models predict O_3 and its response to reductions of precursors correctly and without compensating errors, so that they can be used to develop cost-effective emission control strategies for demonstrating attainment of the O_3 ambient air quality standards.

CONCEPTUAL MODEL

The conceptual model is a qualitative compilation of the physical and chemical processes that govern the formation of O_3, which, to the extent possible, is supported by quantitative information. Two scenarios help conceptualize the dynamics and chemistry of O_3 pollution in the SJV: (1) transport of O_3 and precursors from upwind areas into the SJV, and (2) precursor emissions, O_3-forming reactions, and pollutant transport processes within the SJV. The influence of O_3 and precursors from upwind areas is enhanced by organized flow from the north/northwest into the valley. During multi-day stagnation periods, within-valley processes of particular importance are emissions and transport processes including, but not limited to, eddy patterns, nocturnal jets, recirculation of polluted surface layers due to terrain-restricted outflows, large-scale subsidence events, and vertical mixing. These two scenarios are neither mutually exclusive nor collectively exhaustive.

Transport of O_3 and Precursors from Upwind Areas into the SJV

O_3 and precursors from point, area, and mobile sources accumulate in the mixed layer during the day in the San Francisco Bay area, where mobile sources account for > 50% of the VOC and NO_x emissions. The pollutants are distributed throughout the mixed layer by turbulent diffusion. Some elevated point sources may be released above the mixed layer, and these tend to remain as intact plumes for longer periods of time. When synoptic conditions are favorable, daytime sea breezes are funneled through the Carquinez Strait and nearby mountain passes, bringing O_3 and precursors into the northern part of the SJV by low-level advection. Some inflow is also observed through the Pacheco Pass to the west side of the SJV. Fluxes of O_3 and NO_x accompanying sea breezes can be significant, as measured during the SJVAQS/AUSPEX program. While VOC fluxes were not directly measured during the 1990 study, both fresh and aged VOC (e.g., from traffic in and out of the Bay Area) are expected to reach the Central Valley along with O_3 and NO_x. These transported pollutants contribute primarily to high O_3 in the northern part of the SJV in the late afternoon and may be distributed to other parts of the SJV overnight (see discussion under long-range transport).

Except for terrain-induced vertical motions of air through mountain passes, vertical processes are of little relevance in this transport phenomenon. August 6, 1990 was an example when onshore flows became more dominant after the synoptic high pressure system moved away from the SJV.[7] High O_3 concentrations were observed in the northwestern SJV (120–150 ppb near Tracy/Stockton and Crows Landing) in the late afternoon. Since the morning aloft (carryover) O_3 was only 40–50 ppb, the afternoon peak was consistent with the influence of pollutant transport from the Bay Area. In addition, pollutant fluxes from the Sacramento Valley exacerbated the problem. The combined NO_x fluxes into the northern part of the SJV exceeded the northern valley emissions on that day.[8]

Precursor Emissions, O_3-Forming Reactions, and Pollutant Transport Processes within the SJV

Although the transport of O_3 and precursors from upwind areas contributes to O_3 accumulation in the SJV, the within-valley production of O_3 was postulated to be capable of generating O_3 levels that exceed the NAAQS.[9] O_3 formation in the valley results from an interplay of chemistry with physical processes including emissions of precursors (NO_x and VOC), aloft long-range transport within the valley, vertical mixing under the large-scale subsidence, and deposition.

Emissions and Concentrations of NO_x and VOC in the SJV. According to SJV emissions inventories, the major NO_x contributors are mobile sources,[10] consistent with observations of maximum morning concentrations of NO_x in urban areas. Elevated point sources most likely influence O_3 production farther downwind than surface emissions, except under meteorological conditions conducive to downwash near the stacks.[11] The chemical mass balance (CMB) results show VOC contributions from vehicle exhaust, liquid gasoline, gasoline vapor, oil production, and acetone and unidentified/unexplained VOC. During the 1990 field study, VOC concentrations were highest in the morning samples from the southern SJV, where significant hydrocarbon emissions occurred from oil production. Motor vehicle exhaust was the main contributor at all time periods in the urban areas, ranging from 35 to 70% of total VOCs.[12]

Compared to the CMB results, inventory estimates of motor vehicle VOC emissions (exhaust and evaporation) were significantly lower. The emissions inventory would need to be increased by factors of 3 to 4 to be consistent with the observed ambient concentrations at urban sites.[12] The Yosemite and Sequoia sites showed 10–15% VOC contributions from biogenic emissions according to the CMB results. However, the inventory estimates were substantially higher (> 50%). This discrepancy may be due to the transport of VOC (anthropogenic emissions and secondary organic compounds) from urban areas, the high reactivity of isoprene, or uncertainties in the biogenic emission estimates. Larger unidentified VOC and acetone fractions were measured in the afternoon samples than in the morning samples, reflecting the O_3-producing atmospheric reactions that took place during the day. Same-day urban-scale production resulted in high O_3 downwind from urban centers (e.g., Fresno, Bakersfield) in the late afternoon.

Aloft Long-Range Transport within the SJV. Ground-level winds are generally weak. Long-range transport takes place aloft, particularly at night, when a nocturnal jet develops approximately along the axis of the SJV at an altitude of about 400 m. The nocturnal jet carries pollutants toward the southern tip of the valley (up-valley) at 10–30 m sec^{-1}. By early morning, the Fresno eddy forms due to blockage by the elevated terrain. Eddy flows recirculate transported pollutants in the southern SJV, and as they collapse, early morning emissions in Fresno and Bakersfield are also recirculated in the source area. Aloft concentration data show that the carry-over burden of O_3 increases from the northern part of the SJV to the southern part and is as high as 100 ppb in the downwind area, where the highest O_3 concentrations are observed.[8]

Similar to the characteristics of precursors in the afternoon, aloft parcels contain little NO_x, and the VOC mixture tends to be chemically aged, with concentrations of about a quarter of those measured at ground level in the morning. Long-range transport appears to be especially important in influencing the O_3 concentrations at rural sites with no significant sources nearby. (Note that air exchange between the southwest SJV and the San Luis Obispo area–for example, over the Cholame Pass–may result in high O_3 in either area under different synoptic-scale meteorology.[4]) With efficient transport by the nocturnal jet, sources hundreds of miles upwind may contribute to high O_3 concentrations in the southern part of the valley when the aloft air is mixed into the surface layer during the next day.

Vertical Mixing. The large-scale subsidence from the East Pacific Ridge and the advection of warm, rather moist air from the southeast keep the mixed layer shallow (400–1200 m), despite high temperatures (40 °C). Reduced mixing is a major factor contributing to pollutant buildup. Pollutants within the daytime mixed layer may be trapped above the surface layer at night (< ~100 m). Insulated from ground-level emissions, aloft O_3 can be preserved overnight. O_3 at elevated sites such as Sequoia may stay above 70 ppb at night (e.g., August 2, 1990[2]), an indication of the extent of O_3 preservation aloft. Some point sources have high enough buoyancy at night to carry pollutants to and above the inversion layer as a coherent plume before cooling to the ambient nighttime temperature. Preserved O_3 and other pollutants are transported downwind by the nocturnal jet.

In the morning, under the strong insolation, the temperature rises rapidly, forming a mixed layer that brings the transported pollutants to the surface. Since the aloft air is characterized by high O_3 concentrations in many parts of the SJV, the immediate effect of vertical mixing in the morning may be the titration of surface NO by O_3 to form NO_2. As the mixed layer grows, O_3 production may take place both at the surface and aloft within the mixed layer. At present, the extent of O_3 production aloft is uncertain. The relative efficiency of photochemical reactions at the surface and aloft may be related to the light extinction characteristics of PM.[13,14] For example, UV reductions associated with high aerosol loadings can result in a decrease in O_3 of several percent due to the absorptive properties of nitrate and aromatic aerosols.[13]

Upslope circulation along the Sierras and the Coastal Range generates divergence in the valley, strengthening the subsidence and keeping the mixed layer shallow. The pollutants are therefore trapped in the valley, without much possibility of escape except over the Chalome Pass (west side of the SJV, northern boundary of Kern County) and the Tehachapi Pass. Dry deposition, especially over agricultural land, appears to be an important physical removal process for O_3 within the SJV. However, dry deposition of precursors and products has not been thoroughly studied.

Sensitivity of O_3 to Precursors

Computer modeling and data analyses using observation-based models show that summer O_3 in most areas of the SJV appears to be more sensitive to NO_x controls than to VOC reductions alone.[15,16] However, there is significant evidence that summer O_3 in the San Francisco Bay area is VOC-sensitive. In fact, reductions in NO_x may result in an increase in O_3 in the Bay Area.[15,17-19] O_3 sensitivity is a function of location and meteorology. Major urban centers in the northern SJV may be VOC-sensitive, although other parts may be NO_x-sensitive.[15] Since slight O_3 reductions in the northern SJV result from NO_x reductions in the Bay Area under certain meteorological scenarios,[15] Bay Area emissions contribute to NO_x budgets in the SJV, and the northern SJV may be the transition location where the Bay Area air mass changes over from VOC to NO_x sensitivity as it travels downwind.

Key Knowledge Gaps Identified by the Conceptual Model

In the formulation of a conceptual model for O_3 formation in the SJV, several knowledge gaps were identified. Of the most significant consequence is the sensitivity of

O_3 chemistry at different receptor locations for different meteorological scenarios. Lu and Chang[16] studied the response of SJV O_3 to domain-wide reductions in NO_x and VOC emissions and found that the SJV is NO_x-sensitive for the August 4–5, 1990 scenario. However, the northwestern SJV may be influenced by Bay Area emissions when sea breezes penetrate into the valley (e.g., August 6), and by within-valley emissions under more stagnant conditions (e.g., August 4, 5). The sensitivity of O_3 to its precursors under the enhanced transport meteorological scenario has not been verified. The sensitivity of O_3 in the northern SJV depends on the origin of O_3. If O_3 is formed in the Bay Area and transported downwind into the SJV, it will probably exhibit VOC sensitivity.

As a polluted air mass travels downwind, NO_x is depleted faster than VOCs, and O_3 production within the air parcel becomes increasingly NO_x-limited without fresh emissions of precursors. If O_3 is formed downwind from the source area, it may be NO_x-sensitive. The precursor NO_x may be locally emitted or originate from an upwind location. The more likely scenario is that the observed O_3 in the northern SJV is a combination of O_3 produced upwind and in the SJV. In this case, while VOC controls in the San Francisco Bay area may be beneficial for reducing O_3 production in the Bay Area and transported O_3 at the receptor sites in the northern part of the SJV, NO_x controls may be needed within the valley to reduce the O_3 production potential in areas affected by both fresh emissions and aged air from the Bay Area.

Eight-hour average concentrations of O_3 exceed 80 ppb at many urban and rural sites (see Figure 3). Rural sites may be affected by aloft transport of O_3 and precursors from upwind areas, vertical exchange with the surface layer and free troposphere (especially for elevated sites such as Yosemite), local production of O_3 from biogenic emissions, and O_3 scavenging by reactive VOCs. The processes/fluxes contributing to high 8-hr concentrations at rural sites have not been fully elucidated. The sensitivity of O_3 to precursors may also be different for the 8-hr average concentrations, so that the current understanding of 1-hr sensitivities cannot be translated to 8-hr average O_3 with certainty.

Other knowledge gaps include the extent of aloft production of O_3 and the importance of deposition of precursors and product species other than O_3. Since the conceptual model was formulated primarily based on information from the 1990 SJVAQS/AUSPEX episodes, the representativeness of the meteorology of those episodes needs to be confirmed.

ASSESSMENT OF THE METEOROLOGICAL MODEL MM5

In SARMAP, the mesoscale meteorological model (MM5) was used to simulate meteorology in the SJV. We evaluate the extent to which the simulations of the SJV agree with the available data and examine whether there are weaknesses or deficiencies in MM5 that preclude it from representing the conceptual model presented above. This evaluation is based primarily on the work of Seaman et al.[7] and Seaman and Stauffer.[20] We also draw on our experience with MM5 simulations performed for other purposes, mainly over the Los Angeles basin,[21] the Tennessee Valley,[22] and the New England states.[23]

MM5 is a non-hydrostatic mesoscale model developed at the Pennsylvania State University and the National Center for Atmospheric Research (NCAR).[24,25] The model can run in nested mode, with one or more fine mesh inner grids communicating with a coarser mesh outer grid. This approach makes it possible to perform very fine resolution simulations on a small area without undue influences from the lateral boundary conditions, which need to be imposed only on the outermost grid. MM5 includes a complete set of physical parameterizations, and includes several types of parameterizations for each physical process. A four-dimensional data assimilation (FDDA) system is also available for MM5. It is a Newtonian relaxation, or “nudging,” system, in which an extra term is added to the tendency equations. This extra term is proportional to the difference between the model solution and the observations or a large-scale analysis.

Seaman et al.[7] performed simulations with a triply nested grid, with the inner grid covering the entire SJV with a horizontal mesh size of 4 km and a vertical resolution of 30 layers (ranging from 20 m to 1 km) from ground level to the tropopause. Overall, the MM5 simulations of the SARMAP episodes are quite good, especially the runs that assimilate the special observation data. All the important meteorological aspects of transport in the SJV are qualitatively well simulated by the model. These include the sea breezes, the funneling of the flow through the Carquinez Strait and the other openings of the Coastal Range, the upslope flow during the day along the Coastal Range and the Sierra Nevada, the nocturnal jet along the valley axis, and the Fresno eddy. Although these simulations are generally successful, we discuss below several aspects that could be improved.

Domain and Resolution

One of the main deficiencies of the meteorological simulations is the inability of the model to split the flow east of the Carquinez Strait in the highest resolution domain. Normally, the low-level flow should split into two branches, one going southeast up the SJV and the other one turning north up the Sacramento Valley. The northern part of the flow is generally absent in the high-resolution domain, although there are indications of the flow in the lower resolution domains. There is evidence that this problem is related to the position of the northern boundary of the domain. In one simulation where the inner domain was enlarged to include part of northern Sacramento Valley, the split of the flow was much better simulated.

The strength of the wind through the Carquinez Strait and Altamont Pass, east of the San Francisco Bay, is generally too weak in the MM5 simulations, because of the lack of resolution of the very small-scale topography that funnels and accelerates wind through the pass. This limitation could be overcome by increasing the resolution of the model at the expense of computational resources. While the inability to simulate the peak wind may result in an inaccurate transport time between the San Francisco Bay area and the SJV, the observed high velocities are characteristic of very small areas. The total flux of material through the straights and passes is probably more accurately simulated than the maximum wind. It is the wind-induced stretching of the air parcels and the resulting mixing of pollutants that are not well simulated by the model.

Data Assimilation

The data assimilation procedure used in the MM5 simulations is nudging toward a combination of large-scale analysis and special observations. The Cressman scheme used in this case is of the successive correction type, which is fairly primitive and cannot easily take into account the specific error characteristics of different observing systems. Seaman and Stauffer[20] argue against using the more sophisticated optimal interpolation method because of the lack of appropriate error covariance matrices. These error covariance matrices are now available,[26,27] and can be used to incorporate various types of data (such as radiosondes, profilers, or satellite retrievals) with the proper weights, using optimal interpolation.

Surface observations of temperature were not assimilated using the Blackadar planetary boundary layer (PBL) scheme (see below) because the diagnosed PBL height, which is a critical input to the scheme, is very sensitive to the surface temperature. Nudging toward a higher or lower temperature can easily result in an unrealistic deepening or collapse of the PBL. This problem could be reduced by using a scheme (such as the Gayno-Seaman [G-S] scheme discussed below) in which the PBL structure is less sensitive to the surface temperature. The assimilation of surface temperature observations will likely improve the simulations.

Errors in the PBL height in the San Francisco Bay area may be due to the lack of meteorological data to the north and east of the region. Adequate data coverage extending beyond the limits of the region of interest should be considered in future studies.

Treatment of Processes

The two most important parameterization schemes used for these simulations are the radiation scheme and the PBL scheme. There was no large-scale precipitation and little moist convection during the period; therefore, the cloud and precipitation parameterizations could not be tested. The radiation scheme used by Seaman et al.[7] was a surface energy balance computed with a uniform cooling rate throughout the atmosphere. The transfer of radiation between atmospheric layers was not represented. This scheme is sufficient to simulate the first-order effects of radiative transfer, but does not reproduce accurately the details of atmospheric heating and cooling. In particular, the cooling of the PBL at night tends to be underestimated. The radiative cooling of the marine boundary layer as it moves beyond the San Francisco Bay area toward Sacramento is also poorly simulated by the model. Surface layer temperatures are 4–6 °C too high in this area. A more complete radiation scheme[28] is available for MM5, but it makes the computation slightly more expensive.

Two different PBL formulations were used in Seaman's simulations. The first one was Blackadar's first-order scheme.[29] The other was the G-S higher-order scheme,[3] which can also handle fog, including its radiative effects. (Fog is not important for explaining the summertime O_3 formation, although it would be relevant to wintertime simulations in the SJV.) Both schemes rely on the diffusion equation to exchange heat and momentum between model layers, with small differences in the calculation of the diffusion coefficients. The Blackadar scheme calculates diffusion coefficients from the thermodynamic structure of the atmosphere, while the G-S scheme relates them to the predicted turbulent kinetic energy. Overall, the G-S scheme performed marginally better than the Blackadar scheme, except that the time of maximum wind speed in the lowest model layer was 1–2 hr later than observed.

Due to the lack of data, the initialization of the ground temperature and moisture is a problem common to all weather forecast models. Since the soil has a large heat capacity and moisture retention capacity, errors in the initial specification (up to 5 layers of soil need to be represented) can affect the simulation over several days. Seaman and Stauffer[20] suggest that an overestimation of the deep soil temperature may contribute to the overprediction of surface temperatures at night in some areas. It would be helpful to measure these quantities during intensive observation periods, but the large variability of soil types makes it difficult to develop a proper measurement strategy.

The vertical and horizontal diffusion schemes of the model are important for winds, heat, and water vapor. The diffusion coefficient depends on the Richardson number and is generally small, but has a minimum value to ensure numerical stability. This minimum diffusion coefficient needs to be carefully set (as low as 0.01 m^2/sec) to avoid unrealistic smoothing of vertical profiles, such as the sharp discontinuity in the nocturnal inversion. The horizontal diffusion scheme has little physical basis, besides being of the fourth order and therefore fairly strongly scale-dependent. It is used mainly for numerical stability. We are not aware of any detailed studies of the effects of horizontal diffusion in MM5.

All meteorological models, including MM5, have more difficulty forecasting calm conditions than situations when the dynamic forcing is very strong, during which the dominant terms of the equations of motion are the advection terms, which can be computed relatively accurately. Under calm conditions, the diabatic terms (radiation, turbulence, convection) are dominant. Since these terms are simulated with parameterizations that are far from perfect, meteorological models tend to perform less satisfactorily under calm conditions. In terms of simulating pollutant concentrations, the critical quantity in calm conditions is the evolution of the height of the boundary layer. During the daytime, the height of the convective boundary layer governs the concentrations of pollutants, which are nearly well mixed within it. Under appropriate conditions, cumulus convection can develop, venting boundary layer pollutants into the free atmosphere. This phenomenon was not significant during the episodes studied. Venting also happens at night to some extent when the boundary layer height collapses because of cooling of the surface.

In the SJV episodes, the remnant of the polluted upper boundary layer tended to be transported up-valley by the nocturnal jet. In the numerical experiments of Seaman and Stauffer, the boundary layer height was somewhat overestimated by the model because the upper level subsidence was a little too weak. This would tend to mix pollutants in a deeper layer than observed and would result in slight underpredictions of concentrations in the source area, which may have been counterbalanced by the larger vertical extent of the low level jet due to smoother model profiles. As a result, approximately correct net transport was predicted.

ASSESSMENT OF THE AIR QUALITY MODEL

While SAQM is being reviewed here, many of the comments in this section are generally applicable to other state-of-the-art modeling platforms, such as Models-3. SAQM is a three-dimensional regional-scale air quality model.[31] It is based on the modeling framework of the Regional Acid Deposition Model (RADM), with the most fundamental difference being the reformulation of the model to use non-hydrostatic meteorological data. SAQM takes as inputs emissions data, meteorological data (output from MM5), and initial/boundary conditions, and simulates the chemical and physical processes relevant to O_3 formation. Cloud processes are ignored in SAQM (the RADM submodule was bypassed) because of the general lack of clouds (or fogs) during O_3 episodes. SAQM, as developed under SARMAP, does not treat aerosol formation, since aerosols were not prevalent in the SJV during the summer O_3 season. Recent evidence[13,14] shows that particles may affect solar radiation and indirectly affect O_3 production at the surface. Therefore, aerosol processes and properties, especially the feedback between aerosols and irradiance, may very well be a necessary development in SAQM. We discuss below some aspects of the SAQM formulation that may warrant improvements for future applications.

Domain and Resolution

The SJV is affected by O_3 and precursors from the San Francisco Bay area and the Sacramento area under certain meteorological conditions. In addition, air exchange also takes place between the southern SJV and the San Luis Obispo area.[4] Polluted air exits the SJV primarily through the Tehachapi Pass. The modeling domain used in the Air Resources Board (ARB) simulations[32] extends from just north of the Sacramento metropolitan area to the Tehachapi Mountains in the southeast corner, and includes the upwind coastal cities on the west. To properly simulate all the advective fluxes, a modeling domain that includes the entire Sacramento Valley (up to Redding in the north) and extends farther east beyond the Tehachapi Pass is desirable. Because of the continuous influx from the Pacific, Dabdub et al.[33] found that 4 times as much NO_x originates from the upwind boundary than within the SJV. Aircraft measurements have shown that the polluted air mass can extend for several km offshore, with an estimated NO_x boundary condition of 3 ppb.[33] Extending the western boundary to properly simulate land/sea breezes and the recycling of pollutants may reduce some of the influence of pollutants from the boundary. However, the recommendation for the exact location of the boundary will require better characterization of the cycling of pollutants due to land/sea breezes. Clean air boundary conditions may not be valid even when land/sea breezes are properly simulated, because of intercontinental transport of O_3 and PAN.

Berntsen et al.[34] calculated, using a global model, that mean contributions of about 4 ppb O_3 and 26 ppt PAN in the northwestern United States can be attributed to Asian sources. The intercontinental influence is expected to increase with the increase of Asian anthropogenic emissions in the next decades.[35] In light of the effects of the upwind boundary conditions, offshore measurements are required to define the upwind background.

In previous studies, SAQM was applied with coarser resolution (12 km over the entire domain except for 4 km nested grids in urban areas) than MM5. As a result, meteorological model outputs have to be spatially averaged when used as inputs to air quality models. The processing of meteorological fields may introduce inconsistencies in the flow fields, which necessitate mass adjustment in the air quality model in areas with significant vertical transport.[36] For a regional domain such as the Central Valley, decreasing the grid size to be commensurate with the meteorological model over the entire domain may be infeasible for an air quality simulation because of the associated computational cost. Therefore, it is important to ensure the consistencies of flow fields when using meteorological model outputs to drive air quality simulations.

Despite high surface temperatures in the summer after noon, the mixing layer within the SJV tended to be fairly low (400–1200 m). At night, NO surface emissions scavenge O_3 near the ground but are isolated from the O_3 aloft due to the surface inversion. A high model resolution (tens of meters) near the surface is necessary to properly simulate the processes within this surface layer. A surface layer submodel (SLS) is included in SAQM to provide finer resolution close to the surface (to match the resolution of the lowest level of MM5, with three layers in the first 60 m). Unfortunately, it was found in an application of SAQM to the Los Angeles Basin that, while predictions of O_3 at night are improved by the use of SLS, the performance of the model during the day and for other pollutants is unsatisfactory.[37] For example, the concentrations of NO and NO_2 were seriously overpredicted during the day in the bottom layer. A thorough evaluation of the SLS is needed to identify any possible implementation flaws and/or other compensating errors in the model.

Treatment of Processes

Emissions. Emission sources handled by SAQM include area and point sources. The vertical location of point source emission inputs is determined by the effective stack height of the source, estimated by the plume rise module of the emission pre-processor. It may be preferable to calculate the plume rise internally in SAQM to ensure the consistency of the meteorological fields (e.g., wind speed at stack height) used in the plume rise calculation and those used in simulating other processes (e.g., advective transport in the layer corresponding to the plume height). The chemistry of SO_2 and NO_x differs significantly in point source plumes and in the background for area emissions.[38-40] To that effect, SAQM contains a sub-grid- scale treatment of plumes from large point sources.[41] Plume-in-grid treatments have been applied to sources in the Bay Area, and their effects on O_3 predictions were found to be small. However, the algorithm is unsatisfactory in its treatment of plume dispersion, wind shear, plume overlapping, and effect of turbulence on chemical reaction rates. Newer plume-in-grid models[42] are available that overcome these limitations. Such a model is being incorporated into the Models-3 framework and should be incorporated into SAQM to better simulate major SO_2 and NO_x plumes from refineries near Bakersfield and NO_x plumes from fossil-fuel fired power plants until they reach a size commensurate with that of the grid cells.

Transport by the Mean Wind. The numerical treatment of transport is particularly important for regional-scale applications due to low concentrations of chemical species in rural areas. At surface wind speeds of < 2 m/sec observed during the SJVAQS/AUSPEX, it is essential that numerical errors be minimized in the advection scheme. Bott's scheme, used in SAQM, has undergone rigorous testing and was shown to treat low concentrations with great accuracy.[43] It is expected to be less susceptible to numerical diffusion than the Smolarkiewicz scheme it replaced. However, significant upstream numerical diffusion has been observed in some applications of Bott's scheme.[22,44] New advection schemes may help reduce numerical diffusion problems.[45,46] In addition, further testing and development work may be needed for applications involving low wind speeds. Reducing the grid size may be one way to reduce numerical diffusion during stagnation.

Vertical Mixing. Vertical mixing involves turbulent diffusion, convective mixing, and relief-driven upslope and downslope flows. Accurate representations of meteorology (e.g., wind speeds, temperature profiles, mixing heights, and surface heat fluxes) are necessary for the accurate prediction of vertical transport, particularly in locations with complex terrain. However, the processing of MM5 meteorological fields results in mass consistency problems in areas of high vertical transport, as discussed previously.

It seems intuitive that MM5 and SAQM should use the same method to calculate the vertical eddy diffusivity (K_z) fields used to simulate sub-grid-scale turbulent dispersion, since the turbulent eddies responsible for the dispersion of heat, momentum, and water vapor in MM5 are also responsible for the dispersion of pollutants in SAQM. However, as currently formulated, SAQM estimates the K_z fields internally, and these fields could be different from those estimated by MM5. The computational significance of different K_z predictions in MM5 and SAQM may be tested by modifying SAQM to receive external K_z values from MM5 simulations.

Gas-Phase Chemistry. SAQM was designed to be used with either the Statewide Air Pollution Research Center (SAPRC-90) mechanism[47] or the Carbon Bond Mechanism, version 4 (CBM-IV).[48] Both SAPRC[49] and the current version of CBM-IV have been updated with revised isoprene chemistry. In light of the abundance of biogenic emissions in the inventory[9] and the high reactivity of these compounds, the more current versions of the mechanisms will provide more accurate descriptions of the chemical processes within the SJV.

In the conceptual model, we discussed the NO_x sensitivity of the O_3 system in the SJV and the VOC sensitivity in the San Francisco Bay area. Therefore, it is important that the chemical mechanisms properly simulate both NO_x- and VOC-sensitive regimes in terms of O_3; precursors VOC and NO_x; other products, such as HNO_3, PAN, and H_2O_2; and the radicals OH, HO_2/RO_2, and NO_3. The results of the SAQM/SAPRC and SAQM/CBM-IV models should be compared for consistency for both NO_x- and VOC-sensitive chemistry.

Deposition. Dry deposition is simulated in SAQM using the resistance-in-series approach. The dry deposition module in SAQM was reportedly updated[32] based on findings from the California Ozone Deposition Experiment.[50] Massman et al.[50] found that RADM, the precursor of SAQM, overpredicted the deposition velocity of O_3 for two types of plant cover and incorrectly partitioned O_3 fluxes between transpiring and non-transpiring components of the third site. A recent process analysis comparison[36] found that SAQM predicted higher deposition fluxes than other models, which seems inconsistent with the modifications reported in DeMassa et al.[32] Since dry deposition is potentially an important mass flux in the SJV, especially in rural areas, any inaccuracy of the model representation needs to be understood and rectified.

DATA AND MODEL DEVELOPMENT NEEDS

Field Measurements

Field data needed to support model application and evaluation have previously been compiled by Seigneur et al.[51] Additional data needed to improve the conceptual model or to evaluate key aspects of the MM5/SAQM modeling system are presented below.

A key knowledge gap is the sensitivities of O_3 to VOC or NO_x as a function of location, meteorology, and season. Evidence indicates that the San Francisco Bay area is in a VOC-sensitive regime during summertime, while most of the SJV appears to be more sensitive to NO_x. The sensitivities of O_3 to its precursors in the northern part of the SJV may alter as a result of increased transport from the San Francisco Bay area. Analyses are also needed for areas that may experience 8-hr averaged O_3 concentrations above 80 ppb. In addition to measuring the relevant indicator species (e.g., HNO_3 + nitrates, H_2O_2 + organic peroxides, NO_y), a more comprehensive evaluation of the indicator approach[52] under different meteorological scenarios is desirable. Oxidant chemistry may change from being NO_x-sensitive in the summer to VOC-sensitive in the winter.[53] Pun and Seigneur[54] hypothesized that the wintertime formation of PM NO_3^- and HNO_3 may be limited by the availability of oxidants, which may be VOC-sensitive. A holistic approach to air pollution control (O_3 in the summer and PM in the winter) requires a comprehensive understanding of the chemistry in both seasons.

Solar radiation measurements are needed at the surface and aloft, to evaluate photochemistry as a function of altitude, and to investigate the effects of particles, if any, on the production of O_3. Dry deposition fluxes of precursors and products are needed to provide a better understanding of the pollutant removal processes within the valley. Measurements of deposition fluxes of NO, NO_2, HNO_3, PAN, and VOC are needed over a range of surfaces and atmospheric conditions.

In terms of data for model application and evaluation, meteorological data (surface and aloft winds, temperature, relative humidity, mixing height) in an area extending beyond the area of interest, especially in the regions where strong advection may be expected, would be used with FDDA in MM5 to better characterize mesoscale wind flow patterns that extend to the edges of the air quality modeling domain (e.g., flow up the Sacramento Valley from the flow divergence that occurs east of the Carquinez Strait). It would also be useful to obtain measurements of ground temperature and moisture or surface fluxes at various points throughout the domain. Note that, while the surface albedo is fairly well known from satellite observations, the soil heat capacity and moisture diffusivity, which are important in computing surface fluxes, are quite variable from point to point and are poorly known. This information could be used in evaluating the causes of surface temperature overprediction by the model. The radiative effects of aerosols have also been completely ignored in the model simulations, and could also affect the surface and boundary layer temperature predictions.

During SJVAQS/AUSPEX, the NO_x and NO_2 measurements suffered from interference from oxidized nitrogen species such as PAN and HNO_3. Accurate measurements of nitrogen species, especially NO_x, NO_2, and PAN, are important both for the understanding of the characteristics of air masses of different chemical "age" and for diagnostic model evaluation purposes.

NO_3 measurements were taken during SJVAQS/AUSPEX. The concentrations of NO_3 in the SJV were sufficient to oxidize organic compounds at the same rate in the evening as they were oxidized by OH during the day.[55] Typically, VOC oxidation at night by NO_3 is expected to be two orders of magnitude slower than the daytime process initiated by OH.[56] Smith et al.'s unexpected conclusion shows that it is important to measure other radicals in addition to NO_3, especially OH, HO_2, and RO_2, which have never been measured in large-scale field programs in the SJV, and to use this information in diagnostic model evaluation.

In addition to these new measurements, we recommend further improvements in the following in terms of spatial, temporal, or species resolution:

- The emission inventories (NO_x, VOC, etc) should be refined for biogenic, mobile (e.g., weekday vs. weekend inventories, CMB contributions vs. inventories), oil production, and uninventoried sources.
- More aloft concentration data (O_3, speciated VOC, NO, NO_2, NO_y) should be collected to allow for model evaluation of aloft processes.
- Concentration data (O_3, NO_x) are needed for specification of the boundary concentrations at the upwind boundary of the modeling domain. (Clean air concentrations should not be assumed at the western edge of the domain due to the recycling of the polluted air mass and the influence of intercontinental pollutant transport.)

Model Development

Specific areas needed for MM5 model development include (1) using optimal interpolation to assimilate various types of data with different error characteristics, (2) reducing as much as possible the numerical diffusion by using better algorithms, and (3) using a full radiation scheme and a PBL scheme that is not overly sensitive to surface temperature.

Specific areas of SAQM model development include (1) incorporating the effect of aerosols on solar radiation and photolysis reactions, (2) implementing an advanced sub-grid-scale treatment of plumes, (3) evaluating the performance of the dry deposition module, (4) resolving mass adjustment by modifying the processing procedures of MM5 outputs, (5) improving the surface layer representation, and (6) updating isoprene chemistry. More recent modeling platforms, such as Models-3, contain up-to-date isoprene chemistry and modules to simulate the effects of aerosols on radiative transfer (though typically not the feedback of radiation on aerosol formation). An advanced sub-grid plume model is being developed within the Models-3 platform.

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About the Authors

Dr. Betty Pun (corresponding author) is a staff scientist in the Air Quality Division of Atmospheric & Environmental Research, Inc. (AERI), 2682 Bishop Drive, Suite 120, San Ramon, CA 94583; Dr. Jean-François Louis is principal scientist in the Numerical Weather Prediction Group at AERI, 840 Memorial Drive, Cambridge, MA. Dr. Prasad Pai was a senior scientist in the Air Quality Division; he is currently a program manager at Sun Microsystems, 901 San Antonio Road, Palo Alto, CA. Dr. Christian Seigneur is vice president and head of the Air Quality Division of AERI. Mr. Sam Altshuler is a unit supervisor in Technical and Ecological Services at Pacific Gas & Electric Company, San Ramon, CA. Mr. Guido Franco is an associate mechanical engineer with the California Energy Commission, Sacramento, CA. Dr. Betty Pun can be reached at phone: (925) 244-7125; fax: (925) 244-7129; and e-mail: pun@aer.com.