A statistical approach to ozone forecasting during fire season in the National Parks, Sierra Nevada, California

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ABSTRACT

Observational data from four continuous ozone and weather monitoring sites operated by the National Park Service are used to develop a statistical forecasting model and to estimate the contribution of wildland fires on ambient ozone levels. The impact of fire smoke on these sites is incorporated in the model by using hourly PM2.5 concentrations predicted by a dynamic smoke transport model (BlueSky). Results from the study indicated the occurrence of significant increases in average ozone levels with increasing fire activity. However, the overall effect on diurnal ozone values seemed to be small (~2% of the variability) when compared with the amount of variability attributed to sources other than fire. For the 3 years in the study the increase in ozone that we were able to attribute to fire was less than 0.5 ppb in 95% of the cases and less than 1.6 ppb in 99% of cases.

Key Words: BlueSky, California air-quality standard, pollution, regression models, spline functions, time series,
1. Introduction

Concerns about smoke from large high-intensity and managed low-intensity fires in the Sierra Nevada, California have been increasing during the past decade. Smoke from large high-intensity fires are known to contain and generate secondary fine particles (PM$_{2.5}$) and ozone precursors. High ozone concentrations have been shown to be harmful to plants even in remote regions such as the National forests and Parks in the USA. In addition to fires, fossil fuel consumption in urban areas as well as use of nitrogenous fertilizers in the San Joaquin Valley upwind both contribute to making the National Parks in Southern Sierra region some of the most ozone polluted Parks in the United States (Unger 1978, Grulke et al. 2003). Attributing increases or decreases in ozone to a specific source, such as fire, is a major challenge because it is hard to quantify all sources of ozone variation. Some studies have shown significant correlations between ozone levels and total burned area burned and biomass consumed by fires in the Western United State (Jaffe, et al. 2008). Various process-based models have been developed for forecasting PM and ozone levels in the presence and absence of fires. One such model is the BlueSky Smoke Dispersion Modeling Framework running operationally at CANSAC. Predictions from process based modeled typically do not include estimates of uncertainties which are essential for model evaluation; for attributing significant effects of fires or other sources of ozone and for forecasting with known precisions.

In this article we evaluate a statistical model that is used to forecast next day ozone levels at given sites. The statistical model takes into account some of the known sources of ozone fluctuations, including changes in temperature, humidity, wind speed, wind direction and, during fire season, effects of smoke from fires. Seasonal
patterns of ozone fluctuation characteristic for a given site are incorporated in the model
by estimating background seasonal levels from historic data. Other sources of variation
not directly accounted for in the model - e.g. variability in daily amount of ozone
produced by sources other than fire - are included in the uncertainty measure as random
effect variables. The advantage of a model that is capable of estimating mean effects and
uncertainties simultaneously is that evaluation of model performance is immediate and
predictions are available with specific precision levels.

The statistical model is developed in two stages. In section 3.1 we estimate
background seasonal trends and daily diurnal patterns for each site using 16-26 years of
historic data depending on the site. Next (section 3.2) we study the effects of daily
fluctuations in weather and fire activity on the residual (de-seasoned) ozone series after
removing the long term background seasonal trends and diurnal patterns, as estimated in
section 3.1. Finally, in section 3.3, we develop a statistical autoregressive model for
forecasting next day ozone levels at sites with continuous ozone and weather monitors.

The goodness of fit and the skill of the statistical model in forecasting ozone are
discussed in section 4. It is anticipated that the forecasts from the statistical model can be
used to support decision making by land and air resource managers regarding air quality
and prescribed burns in the Class-I areas of the Sierra Nevada and other sensitive areas.

2. Study sites and data

The study employed long-term observational data from four sites operated by the
National Park Service in the Sierra Nevada of California. Two of the sites, Ash
Mountain and Lower Kaweah, are located in the Sequoia and Kings Canyon National
Park, while the other two, Turtleback and Yosemite Valley, are in the Yosemite National Park. 

At each of these four sites, ozone concentrations were measured with a Thermo Environmental Model 49 UV absorption instrument operated by the National Park Service. The ozone monitor was calibrated at the beginning of each season and checked against a calibrator on a weekly basis. Each site also had a surface weather station that measured standard meteorological variables. Air temperature and relative humidity were measured with a Vaisala temperature and humidity sensor mounted at approximately 2 m in a self-ventilated, louvered shelter. Wind speed and direction were measured with a MetOne anemometer mounted on a 10-m tower. Data are quality controlled and archived on a personal computer.

The statistical analyses performed employed primarily the hourly averaged values of ozone concentrations and meteorological variables at these sites in the past three years (2006-2008) except for Yosemite Valley site that did not have data for 2008. To describe background ozone patterns at these locations, historical ozone data were also obtained which varied in record lengths from 16 years (1992-2007) for the two Yosemite sites to 24 years (1984-2007) and 26 year (1982-2007) for Lower Kaweah and Ash Mountain sites, respectively.

The impact from fire smoke in the region on ozone concentrations at these locations was taken into account by using, as surrogate, PM$_{2.5}$ concentration obtained from the BlueSky model output at the nearest grid point to the four sites. BlueSky is a smoke dispersion modeling framework that combines burn information with models of consumption, emissions, meteorology, and dispersion to yield a prediction of trajectories
and surface concentrations of particulate matter (both PM\textsubscript{2.5} and PM\textsubscript{10}) from managed low-intensity fires, wildfires, and agricultural burn activities (O’Neill et al. 2008).

Currently BlueSky predictions of smoke from wildfires are available daily for many locations in the United States. In California and Nevada, BlueSky Smoke Dispersion Modeling Framework has been implemented by the California and Nevada Smoke and Air Committee (CANSAC, http://www.cefa.dri.edu/COFF/coffframe.php) (Brown et al., 2003) into its operational weather forecast system. The meteorological fields needed for smoke transport and dispersion are provided by real-time regional weather forecasting using the MM5 meteorological model (Grell et al., 1994) at 4 km grid resolution over a domain that covers California and Nevada. The transport and dispersion of PM\textsubscript{2.5} from fire emissions in the region are estimated using the CALPUFF (Scire et al. 2000) and HYSPLIT (Draxler and Hess, 1997) models. We used the predicted PM\textsubscript{2.5} values from BlueSky forecast to characterize the amount of PM produced by smoke from both large high-intensity and managed low-intensity fires in the region. BlueSky forecasts are zero for days with no reported fires. Outputs from other transport models, with the capability to produce spatially and temporally explicit values in real time, may also be used.

There are several advantages of using output from the state-of-art smoke dispersion model output of the PM values as surrogate for fire activities over previous methods. Previous studies (Preisler et al. 2005) make simple, subjective assumptions about fire impact that based primarily on distance from the fires, wind direction and fire size. However, the metric used in the Preisler et al. (2005) was not a forecast and can only be used for quantifying historic fire effects. Additionally, it did not incorporate topography. The BlueSky model incorporates emissions from all fires and the transport of
smoke from distant fires. The model results, however, may contain relatively large errors
due to uncertainties in emissions, meteorological input, and assumptions on dispersion
mechanisms and smoke deposition etc. Despite these limitations, the method of using
BlueSky predicted PM concentrations resulting from wildland and prescribed fires, which
are available in real-time for California and many other regions in US, provides a better
alternative to the distance and wind direction based empirical approach used in similar
studies in the past.

3. Statistical Models

3.1 Estimating background ozone patterns

The long-term historic ozone data were used to estimate background seasonal
trends and diurnal patterns at the four locations. The 24-h and 12-month ozone cycles
were captured by using a semi-parametric additive regression model with periodic spline
functions (Hastie et al 2001). The statement for the statistical model is given by

\[ y = \alpha + s(\text{day}_{\text{in}_{\text{year}}}) + s(hr) + \varepsilon \]  [1]

where

- \( y \sim \) is the hourly ozone level;
- \( \alpha \sim \) is the intercept parameter;
- \( s(\cdot) \sim \) non-parametric periodic spline function;
- \( \varepsilon \sim \) is a random error term.

A separate equation was estimated for each of the four sites. Non parametric
splines are useful in particular when relationships are not expected to be linear. Period
tspline functions provide a flexible method for fitting relationships with a cyclical pattern
such as the 24-hr diurnal pattern or the 365-day seasonal patterns often seen in ozone values. We also estimated the between year standard deviation that was used later to incorporate between year variability in our overall error bounds. All through our analysis we used the publicly available R statistical package (R Development 2008).

It is anticipated that the estimated background seasonal and diurnal patterns will account for the majority of the natural ozone variability at these locations. The background pattern at each site also reflects the climatological conditions and the averaged ozone exposures. The estimated historic patterns at each site are used in the next sections to de-season the ozone data, before the second stage of fitting wherein contributions of fires are estimated.

3.2. Quantifying sources of variation

Hourly meteorological data from the surface weather stations at each of the four sites were used to evaluate the simultaneous influence of temperature, humidity, wind speed, wind direction, solar radiation to the diurnal variation in ozone values. The PM$_{2.5}$ concentration values from the nearest grid point from BlueSky model predictions is used as surrogate for the influence of smoke on the site as a result of wildland and prescribed fire activities in the region. The BlueSky predicted PM$_{2.5}$ value would be zero if there are no fires in the region or if there are fires and the site is not in the path of the smoke plume. Although BlueSky output used here is not a predicted ozone value put rather forecasted PM$_{2.5}$ (here on referred to as mpm or modeled PM), it is assumed that if the amount of smoke and PM from surrounding fires increases, the amount of ozone precursors coming from the fires is also likely to increase. Our task here is to quantify the
shape and significance of the relationship between mpm, including lagged values of mpm, and ozone.

We used non-parametric spline functions in a linear regression model to estimate the simultaneous effects of the following explanatory variables: temperature, solar radiation, relative humidity, wind speed, wind direction and mpm. Because wind direction is periodic (with a 360° cycle) we estimated a periodic spline for this variable. After some exploratory analysis with various combinations of mpm, the variable that appeared to show the largest significance, and the one used in the final model, was the median of the mpm values of the previous 48 hours (hereafter referred to as mblue).

The specific autoregressive model used to fit the data was

\[ z_{kt} = \alpha + \sum_m s(X_{kmr}) + \varepsilon_t \]  

where \( z_{kt} \) is the residual series for site \( k \) and time \( t \) after removing the background seasonal and diurnal effects estimated from the historic data; \( t \in \{1, \ldots, T\} \) hrs with \( T = 3 \) years x 365 days x 24 hr; \( X_{kmr} \) is value of \( m \)th explanatory variable at time \( t \) and site \( k \); \( s(\cdot) \) is non-parametric smooth spline or periodic spline function; \( \varepsilon_t = \rho_1\varepsilon_{t-1} + \rho_2\varepsilon_{t-2} + \rho_3\varepsilon_{t-3} + \xi \) is an autoregressive process of order 3 with independent Gaussian error terms.

The autoregressive model of order 3 was found necessary to account for the serial correlation in the data (see goodness of fit analysis in section 4). The program gamm() of the R statistical package was used to fit the generalized additive mixed model in equation [2].

3.3. Forecasting Next Day Ozone Levels
This section is concerned with fitting a predictive model for next day ozone levels at sites where hourly ozone and weather values are available. We used an autoregressive model with historic time series information on hourly ozone values up to the previous day in addition to modeled PM and local weather. The specific time series model used to forecast next day ozone levels for a particular site was as follows

\[ z_t = \beta_1 z_{t-24} + \beta_2 mblue^{1/3} + \beta_3 \Delta \text{temp} + \beta_4 \Delta \text{winds} + \beta_5 \Delta \text{windd} + \epsilon_t \]  \[ \text{[3]} \]

where \( z_t \sim \) the residual series for time \( t \) after removing the background seasonal and diurnal effects estimated from historic data;

\[ t \in \{1, T \} \text{ hrs with } T = 3 \text{ years x 365 days x 24 hr}; \]

\[ z_{t-24} = y_{t-24} - h_{yt} \sim \text{difference between historic average } (h_{yt}) \text{ and previous day ozone level } (y_{t-24}); \]

\( mblue \sim \text{median modeled PM}_{2.5} \text{ value for the previous 48 hrs}; \)

The variable \( \text{temp} \) indicates temperature, \( \text{winds} \) and \( \text{windd} \) denote wind speed and direction.

\[ \Delta \text{temp} = \text{temp}_t - \text{temp}_{t-24}; \quad \Delta \text{winds} = \text{winds}_t - \text{winds}_{t-24} \]

\[ \Delta \text{windd} = \begin{cases} 
1 & \text{if } \text{windd}_t \in \{200 - 275\} \text{ and } \text{windd}_{t-24} \notin \{200 - 275\} \\
0 & \text{otherwise} 
\end{cases} \]

\[ \epsilon_t = \rho_1 \epsilon_{t-1} + \rho_2 \epsilon_{t-2} + \rho_3 \epsilon_{t-3} + \xi \sim \text{an autoregressive process of order 3 with } \xi \text{ independent Gaussian error terms.} \]

\( \beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \rho_1, \rho_2, \rho_3 \sim \text{parameters estimated from the data.} \)

The 24-hr lagged difference in the other two weather variables, relative humidity and solar radiation, were not found to be significant when added to the model in [3].
3. Results and Discussion

The background ozone levels at the four sites, as estimated from the historic data, exhibit strong seasonal cycles (Figure 1). At all four sites, ozone concentrations appear to be lowest on average in winter and highest in summer, with peak values occurring in late summer (August). The two Yosemite sites appear to be less polluted on average (using the ozone metric) than the Sequoia –Kings Canyon sites. The Ash Mountain site in Sequoia National Park appears to have the highest average ozone concentration values that reach the critical level of 90 ppb in the months of July and August. Some of the between site differences may be due to differences in topography, elevation and distance from urban sources.

There were significant between station differences in the estimated diurnal patterns (Figure 2). The Yosemite Valley site shows the largest diurnal amplitude, while Turtleback is nearly flat with only a small diurnal signal. Similar difference in diurnal ozone variation among different sites in the Sierra Nevada was also found by Van OoY and Carroll (1995) in a climatological analysis of ozone data and they attributed the difference to the topographic sitting rather than to the remoteness to urban areas that typically explains large and small diurnal variation in ozone concentration. At Ash Mountain and Lower Kaweah, ozone peaks in late afternoon, while at the Yosemite Valley site, the peak appears to occur around noon.

The overall variability in ozone values, as given by the standard deviation over all sites; hours-of-day and days-of-year, was ±18.5 ppb with a mean of 55 ppb and
coefficient of variation of 33%. Table 1 shows the percentage drop in the variance as various explanatory variables are included in the regression model.
Table 1: Estimated drop in variability of ambient ozone as various sources of variation are added to a semi-parametric statistical regression model.

<table>
<thead>
<tr>
<th>Model</th>
<th>Variables</th>
<th>Drop in variance</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Between sites</td>
<td>15.0%</td>
</tr>
<tr>
<td>II</td>
<td>Site specific seasonal + diurnal trends (historic average)</td>
<td>52.0%</td>
</tr>
<tr>
<td>III</td>
<td>I + local met variables</td>
<td>26.0%</td>
</tr>
<tr>
<td>IV</td>
<td>II + local met variables</td>
<td>8.0%</td>
</tr>
<tr>
<td>V</td>
<td>II + mblue</td>
<td>1.7%</td>
</tr>
<tr>
<td>VI</td>
<td>III + mblue</td>
<td>2.5%</td>
</tr>
</tbody>
</table>

As would be expected, a large portion of the variability in ozone values was attributed to between site variations (15%), possibly due to differences in topography between sites. Background seasonal and diurnal patterns (as described in section 3.1 above) appear to ‘explain’ 52% of the variation and local meteorological variables listed above ‘explain’ 26% of the variability. This indicates that most of the ozone variability may be attributed to ‘average weather’ or climate conditions, while only a small fraction (~8%) of it seems to be due to daily variability in local weather conditions superimposed on the seasonal and diurnal pattern. Fire activity, as measured by mblue, explains an additional 1.7% of the variation in the de-seasoned data and 2.5% of the variation when local weather (but not seasonal trends) was included in the model.

The meteorological variable that appears to have the largest effect on the de-seasoned ozone values was temperature (Figure 3), which is not surprising given the known diurnal variation. The estimated curves in Figure 3 were produced by fitting equation [2] to three years of de-seasoned ozone data from the four sites. Partial effects of solar radiation and relative humidity appear to be small but significant. Wind speeds of
greater than 10 m s\(^{-1}\) appear to decrease average ozone levels, however, the standard
errors are large because of the small sample sizes at high winds. Wind directions from
south and south-west (180-300 degrees) appear to increase ozone levels above the
seasonal levels. Given the locations of these four sites on the western slope of the Sierra
Nevada, the increase in ozone levels with winds from south and southwest suggests the
contributions to ozone concentrations at these sites from transport of ozone precursors
from pollution sources in the Central Valley, especially the heavily polluted cities like
Fresno and Bakersfield in the southern part of the valley.

Finally, there seem to be a small but significant effect of fires as measured by the
increase in ozone levels with increasing values of \(mblue\) (the median amount of modeled
PM levels in the last 48 hrs). On average there appeared to be about 2.76 (SE=0.7) ppb
increase in ozone for each one point increase in the cube root value of \(mblue\ (mblue^{1/3})\).
The standard errors around the estimated curve are large, in particular for larger values of
\(mblue\). There were very few observed cases with \(mblue\) values greater than 1. During the
3 years and the 4 sites included in the study, the maximum observed \(mblue\) value was 7.3
with 95% of the observations being less than 0.4. Consequently, during the 3 years of the
study the observed effect of fire (using our \(mblue\) metric) was less than 0.5 ppb
(4.1*0.4\(^{1/3}\)) 95% of the time and less than 1.6 ppb 99% of the time.

The estimated regression line for forecasting next day ozone values was

\[
\hat{y}_t = hy_t + 0.387 \times z_{t-24} + 3.1 \times mblue^{1/3} + 0.28 \times \Delta temp - 0.06 \times \Delta winds + 0.66 \times \Delta windd
\]

\[
(\pm 0.005) \quad (\pm 0.74) \quad (\pm 0.03) \quad (\pm 0.02) \quad (\pm 0.23)
\]

The average standard error around the forecasted model as given in [3] was ±10.4 ppb.
The particular autoregressive model in equations [2] & [3] was used because the
diagnostic tests of the residuals indicated the need for a third order autoregressive process
(Figure 4). The auto-correlation function of the de-seasoned series shows the amount of
serial correlation between lagged hourly ozone values (Figure 4a). An autoregressive
model of order one (AR1) did not seem to remove all the serial correlations with some
significant correlations persisting at 2 and 3 hour lags in addition to those at 24 hr lags
(Figure 4b). There were no apparently significant serial correlations in the residual series
from the final model in [3] (Figure 4c).

We developed graphs of observed and forecasted ozone values for various periods
of time in order to further assess the skill of the statistical model and to study the
contribution of fires to ozone variability (Figures 5,6). During the period 11 - 22 July
2006 there were many lighting caused fires in Yosemite National Park. On July 20 and 22
(day-in-year 201, 203) there were 3 large fires (>100 acres) with one fire on July 22 that
burned 6031 acres. These fires were detected by the BlueSky model as indicated by the
above zero values of the modeled PM levels at the two Yosemite sites (Figure 5). The
estimated amount of increase in ozone that was attributed to the fires, as estimated by the
model, was a maximum of 0.7 ppb (0.8 – 2.3 ppb). Almost all the observed values were
within the forecasted 99th percentile levels.

On 7th May 2006 (day-in-year=186) there was a fire in Sequoia National Park that
burned 619 acres. This was detected by the BlueSky model as indicated by the above zero
values of the modeled PM levels at the two Sequoia NP sites (Figure 6). For this period
the estimated amount of increase in ozone that was attributed to the fire was a maximum
of 2 ppb (0.5-3.0 ppb). Once more, the 99th percentile of the forecasted values gave a
good coverage of the next day observed ozone levels.

The hourly forecasts may also be used to predict next-day 8-hr moving average
levels. California ambient air quality standard for ozone is 70 ppb for the forth highest 8
hour concentration averaged over three years (http://www.arb.ca.gov/research/aaqs). As
an example we produced predicted 8-hr average levels for three periods in 2008 and for
the Lower Kaweah site in Sequoia National Park (Figure 7). We note that the next day
50th and 95th percentiles of the predicted values appear to give a good fit to the actual
observed levels.

4. Conclusions

We have performed statistical analyses of multi-year ozone and meteorological
data at four sites in Sierra Nevada. Using long-term historical data, we established the
average ozone pattern for each site. At all four sites, averaged ozone pattern shows a
strong seasonal cycle with maximum ozone values occurring in late summer and
minimum in winter. The ozone levels are generally higher at sites in the Sequoia and
King Canyon National Park than those in the Yosemite National Park, suggesting the
importance of transport from the Central Valley to the western slope of the Sierra
Nevada. All sites also show a diurnal ozone cycle, but the amplitudes of the diurnal cycle
vary significantly between sites, possibly due to differences in topography.

The sources for ozone variation are quantified using simultaneous measurements
of ozone and meteorological variables in the past three years. As expected, the majority
of ozone variation at these sites is attributed to temperature variation. It was found that
wind directions from south and southwest appear to increase ozone levels above the seasonal average levels, suggesting that the importance of transport of ozone precursors from the sources in the Central Valley.

To assess the contribution of smoke to ozone variations, we used PM concentrations predicted using a smoke dispersion model that incorporated emissions from wildland and prescribed fires in the region. The statistical analysis detected a small but significant effect of fires on ozone variation. Ozone levels appear to increase on average when fire activity in the region increases, but the overall effect, however, seems to be small compared to variation due to meteorological factors and sources other than fires.

We have demonstrated that accurate forecasts of next day hourly ozone levels may be achieved by using the estimates from a time series model with previous day ozone values, historic average values, expected local weather and modeled PM values as explanatory variables. The model produced forecasting explained 68% of the variability in next day’s diurnal ozone levels. For sites with no historic data, forecasting with estimates from a time series model, with only previous day’s values as explanatory variables, can explain 60% of the variability. Comparisons of the model predictions with actual observed ozone values indicate that the model had considerable skill in forecasting ozone for the next 24 hours using local weather and ozone levels in the previous day.

The statistical model and computer program developed in this study can be implemented to produce forecasts in real time. The forecasts will support decision making by land and air resource managers regarding air quality and prescribed burns in the Class-I areas of the Sierra Nevada and other sensitive areas.
Acknowledgements

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References


Figure Legends

Figure 1: Estimated historic average ozone patterns (black curve) for 1400hrs superimposed on observed values for that hours (grey dots) at four stations. Grey band is 95% CL for between year variability. Dashed horizontal line is the critical ozone level of 90 ppb.

Figure 2: Estimated historic diurnal ozone patterns for the four stations evaluated for two dates (a) 15 May and (b) 15 June. Note that, although the diurnal shapes for each site do not change between the dates, the overall increase between 15 May and 15 June is larger for the Sequoia sites as compared to the Yosemite sites.

Figure 3: Estimated effects (partial residuals) of weather and fire variables on the de-seasoned ozone levels -where historic background levels are remove-. Dashed lines are approximate point-wise 95% confidence limits. Hatch marks at the bottom indicate observed levels of the explanatory variable.

Figures 4: Estimated auto-correlation functions for (a) ozone series with seasonal trends removed (b) residual series from fitting an AR(1) to the de-seasoned data and (c) residual series from fitting the model in equation [2].

Figure 5: Observed (black dots); forecasted 50th (green) and 99th (red) percentile ozone values between July 18 and 25, 2006 for (a) Yosemite -Turtle Back doom - site and (b) Yosemite Valley site. Gray band is the historic average level for the given site. Blue curve at the bottom indicate the fire activity level as measured by the median BlueSky value for the last 48 hours \(25*mblue^{1/3}\). Dashed line at top is the critical 90ppb level.

Figure 6: Observed (black dots); forecasted 50th (green) and 99th (red) percentile ozone values for 4 – 10 July, 2006 at (a) SEKI - Ash Mountain site and (b) SEKI – Lower Kaweah site. Gray band is the historic average level for the given site. Blue curve at the bottom indicate the fire activity level as measured by the median BlueSky value for the last 48 hours \(25*mblue^{1/3}\). Dashed line at top is the critical 90ppb level.

Figure 7: Observed (black dots) and forecasted 50th (blue) and 99th (red) percentiles for 8hrs moving average ozone values for (a) 15- 22 May 2008; (b) 15 – 22 July, 2008 and (c) 14 – 21 September, 2008 at the Lower Kaweah site in Sequoia National Park. The dashed line at 70 ppb indicates the critical 8 hr California ambient air quality standard for ozone.
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