Semi-empirical functions describing the response of short-lived radicals to their driving forces in the WRF/Chem model

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ABSTRACT

Short-lived radicals play a key role in the chemistry of the lower atmosphere. They oxidize pollutants, e.g., carbon monoxide (CO) and methane (CH₄), making them more soluble and therefore easier to remove by wet or dry deposition. Without these radicals, tropospheric pollution would accumulate to much higher levels and have a stronger negative effect on our climate and health. To understand short-lived radicals, i.e., hydroxyl radical (OH), we evaluated them against the environmental and chemical driving factors that, theoretically, should control them. We use a semi-empirical function (SEF) that is linear in log space, whose slopes represent the “normalized sensitivity coefficients”. These coefficients describe how sensitive a radical is with respect to changes in the individual driver, e.g., atmospheric water vapor (H₂O), volatile organic compounds (VOCs), nitrogen oxides (NOₓ), and the ultraviolet photolysis coefficient for NO₂ (J(NO₂)). Using the output from the WRF/Chem model and the sensitivity coefficients calculated from the NCAR Master Mechanism box model, we evaluated the chemical concentrations with respect to the SEF and found a linear relation with a reduction in scatter compared to the correlations with each individual driver. However, multiple correlation lines were identified, and their origins were traced to WRF/Chem’s use of different chemical mechanisms over land, ocean, and near the domain boundaries. Therefore, these correlations may provide a powerful technique for comparing models with one another and with measurements, specifically with field campaign observations (like those of MIRAGE) for evaluating the representation of fast radical photochemistry in three-dimensional chemistry-transport models (such as WRF/Chem).

KEYWORDS: hydroxyl radicals, atmospheric chemistry, photochemistry, WRF/Chem

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1. Introduction

Hydroxyl (OH) radicals play an important role in tropospheric chemistry. OH reacts with trace gases, like greenhouse gases, that have been emitted from the surface and oxidizes these molecules. Due to this oxidation the molecules can become more soluble and able to be deposited through precipitation or dry deposition. This removes them from the atmosphere and shortens the residence time of the molecules in the atmosphere. Since OH is the major oxidant in our ‘self-cleansing’ atmosphere, it is vital to understand the global distribution of this radical.

The OH is being continuously produced and destroyed, with a lifetime of about one second (Jacob, 1999; Lelievel et al., 2004), making it very sensitive to its environmental and chemical drivers. This sensitivity explains the variability of OH concentrations in the atmosphere. Studies have shown that OH concentrations can be estimated through proxy molecules such as carbon monoxide containing radiocarbon (Manning et al., 2005) and methyl chloroform (Logan et al., 1981; Spivakosky et al., 1990; Lelieveld et al., 2004). Because of the variability and difficulty in measuring the atmospheric concentration of OH, three-dimensional models face the challenge of how to evaluate the accuracy of predicting the concentration of this short-lived radical. It is vital that models can successfully forecast OH in order to understand what will happen to our climate as the greenhouse gasses and pollutants increase.

OH concentrations depend on multiple environmental and chemical driving factors that become sinks and sources for this radical. It has been known since the early 1970’s that ozone plays a key role in the production of OH in the troposphere (Levy, 1971; Logan et al., 1981). The primary reaction can be seen below in reactions 1-2.

\[
O_3 + h\nu (\lambda < 320\text{nm}) \rightarrow O(^1\text{D}) + O_2
\]  

(1)
O(1D) + H₂O → 2OH  \hspace{1cm} (2)

We can understand from these chemical reactions that the production of OH relies on the photolysis of ozone (O₃), producing an excited oxygen atom (O(1D)) that then reacts with water vapor. A secondary way in which OH is produced is through combinations of chemical reactions between O₃, hydroperoxy radicals (HO₂), nitric oxide (NO), and nitrogen dioxide (NO₂) shown in reactions 3-4.

\[
\begin{align*}
O₃ + HO₂ &\rightarrow OH + 2O₂ \\
NO + HO₂ &\rightarrow OH + NO₂
\end{align*}
\hspace{1cm} (3) \hspace{1cm} (4)
\]

Nitric oxide is mostly emitted by combustion sources, and produces nitrogen dioxide via reaction 4 and also by reaction 5.

\[
NO + O₃ \rightarrow NO₂ + O₂
\hspace{1cm} (5)
\]

During daytime hours, the NO₂ is broken by ultraviolet sunlight back to NO and ground state oxygen atoms which then make ozone:

\[
\begin{align*}
NO₂ + \text{hv} &\rightarrow NO + O \\
O + O₂ &\rightarrow O₃
\end{align*}
\hspace{1cm} J(NO₂) \hspace{1cm} (6) \hspace{1cm} (7)
\]

Reactions 4-7 occur on the time scale of a few minutes during sunlight periods, and determine the ratio NO/NO₂, the so-called photo-stationary state ratio (e.g. Ridley et al., 1992).

Although OH has many sources, it is lost as fast as it is produced by the oxidation process with volatile organic compounds (VOCs), especially hydrocarbons (reaction 8).

\[
\text{OH} + \text{Hydrocarbons} \rightarrow \text{products}
\hspace{1cm} (8)
\]

Similarly, OH is lost by reaction 9 with carbon monoxide (CO).

\[
\text{OH} + \text{CO} \rightarrow \text{CO}_2 + \text{H}
\hspace{1cm} (9)
\]
From the previous discussion, it is clear that OH concentrations are strongly dependent on \( J(\text{NO}_2) \), \( \text{H}_2\text{O} \), VOCs, and \( \text{NO}_x \). Therefore, we parameterize this dependence with a semi-empirical function,

\[
[\text{OH}] = A \ [J(\text{NO}_2)]^\alpha \ [\text{H}_2\text{O}]^\beta \ [\text{NO}_x]^\gamma \ [\text{VOCs}]^\delta ,
\]

in which each driving factor is included multiplicatively. The exponents in Equation 10 (\( \alpha, \beta, \gamma, \) and \( \delta \)) represent the ‘normalized sensitivity coefficients’ that describe how OH changes with respect to each individual driver. These coefficients were calculated using a theoretical box model.

In a previous study (Rohrer and Berresheim, 2006), OH was plotted against a similar function as Equation 10. Only the photolysis of \( \text{O}(^1\text{D}) \) was used as a driver for the production of OH and was found to possess a strong nearly linear correlation. Using model outputs and measurements, a linear dependence of OH on ultraviolet (UV) radiation is continued to be seen. The research presented here is slightly different; our study incorporates more drivers in the empirical function than accounted for by Rohrer and Berresheim. With the addition of drivers, some of the variability seen before should decrease. For the drivers and OH concentration, we used the output from the Weather Research and Forecasting model combined with Chemistry (WRF/Chem) simulation for the 2006 Megacities Impact on Regional and Global Environment (MIRAGE) field campaign.

2. Method

a. Model Output

The data used in this study were output from the WRF/Chem three-dimensional meteorological and chemical model that simulates regional scale processes (Grell et al., 2005).
WRF/Chem contains two chemical mechanisms to choose from, the Statewide Air Pollution Research Center (SAPRC) mechanism and Carbon Bond Mechanism-Z (CBM-Z). Our data simulation used CBM-Z as the chemical mechanism. The simulation ran from 06:00 UTC on March 6 to March 30 at 06:00 UTC, with output every hour (Fast et al., 2009). This study used the first domain in the model with a 12 kilometer resolution, which encompasses Mexico, a portion of Central America and the Pacific Ocean, Southern Texas, and the Gulf of Mexico as seen in Figure 1.

![Fig. 1. Land mask variable plotted showing area that first domain encompasses. Red is the landmass while blue is the bodies of water in the region.](image)

The initial and boundary conditions for the chemical mechanism in the WRF/Chem regional model are provided by the Model for Ozone and Related Chemical Tracers, version 4 (MOZART-4), global chemistry model containing the MOZART chemical mechanism. Although there are some chemical concentrations, i.e. those of long-lived species, that need to have an initial concentration, the concentrations of the rest of the species are produced within WRF/Chem by the chemical mechanisms available.

### b. Data selection

Data for this study were selected with interest in tropospheric chemistry in remote conditions. This study examines the concentrations of OH, nitrogen oxides ($NO_x=NO + NO_2$), photolysis of
NO₂ (J(NO₂)), relative humidity (RH), temperature (T), height (z), and a list of VOCs that can be found in Table 1. The total VOC contribution is a reactivity-weighted sum that was determined with the concentration for each VOC and reactivity rate (k) with respect to OH, as in Equation 11.

\[
\text{VOCs} = ([\text{voc}_1] \times k_1) + ([\text{voc}_2] \times k_2) + \ldots + ([\text{voc}_n] \times k_n)
\]  

(11)

To calculate k for each VOC, we used the rates given in Zaveri and Peters (1999), using temperature (T) from the model as needed in the reactivity rates.

**Table 1. List of VOCs and their reactivity rates with OH (Zaveri and Peters, 1999)**

<table>
<thead>
<tr>
<th>Species</th>
<th>Symbol in Zaveri &amp; Peters, 1999</th>
<th>Symbol in WRF/Chem</th>
<th>k (cm³ molecules⁻¹ sec⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethene</td>
<td>ETH</td>
<td>ol2</td>
<td>(F(1.0(-28), 0.8, 8.8(-12), 0.0))</td>
</tr>
<tr>
<td>Terminal olefin carbons</td>
<td>OLET</td>
<td>olt</td>
<td>(5.8 \times 10^{-12} \exp(478/T))</td>
</tr>
<tr>
<td>Internal olefin carbons</td>
<td>OLEI</td>
<td>oli</td>
<td>(2.9 \times 10^{-11} \exp(255/T))</td>
</tr>
<tr>
<td>Toluene</td>
<td>TOL</td>
<td>tol</td>
<td>(2.1 \times 10^{-12} \exp(322/T))</td>
</tr>
<tr>
<td>Xylene</td>
<td>XYL</td>
<td>xyl</td>
<td>(1.7 \times 10^{-11} \exp(116/T))</td>
</tr>
<tr>
<td>Isoprene</td>
<td>ISOP</td>
<td>iso</td>
<td>(2.55 \times 10^{-11} \exp(409/T))</td>
</tr>
<tr>
<td>Lumped intermediate</td>
<td>ISOPRD</td>
<td>isoprd</td>
<td>(3.3 \times 10^{-11})</td>
</tr>
<tr>
<td>High MW aromatic oxidation fragment</td>
<td>OPEN</td>
<td>open</td>
<td>(3 \times 10^{11})</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>CO</td>
<td>co</td>
<td>(1.5 \times 10^{13} (1 + .6P_{\text{atm}}))</td>
</tr>
</tbody>
</table>

*Where \(P_{\text{atm}} = 0.8 \text{ atm}\)

The retrieved RH value was given in units of percent, which we converted to units of molecules per cubic centimeter (molecules/cm³) using a conversion equation from Seinfeld (1986). All the chemical species were given by the model in units of parts per million (ppm) which had to be converted to molecules/cm³ as well. The data were selected by applying the restrictions and conditions from Table 2. Concerning ourselves with the tropospheric chemistry
of rural locations, far from urban conditions (i.e., Mexico City), the height was restricted to less than 5km (lower troposphere). The NO\textsubscript{x} values of less than 1 part per billion (ppb) were selected to represent remote conditions. Time was chosen to achieve peak photolysis rates. After applying these restrictions, we were left with approximately 440,000 points available for our evaluation.

Table 2. Restrictions for Data Selection

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height (z)</td>
<td>Less than 5km</td>
</tr>
<tr>
<td>NO\textsubscript{x}</td>
<td>Less than 1ppb</td>
</tr>
<tr>
<td>Temperature (T)</td>
<td>280K &lt; T &lt; 285K</td>
</tr>
<tr>
<td>Time</td>
<td>20:00-23:00 UTC</td>
</tr>
</tbody>
</table>

c. Normalized sensitivity coefficients and SEF mathematical derivation

The normalized sensitivity coefficients mentioned earlier come from the derivation of a one dimensional power function. Equations 12-17 describe the steps to solving for the exponent, n.

\[ y = ax^n \]  \hspace{1cm} (12)
\[ \frac{dy}{dx} = a nx^{n-1} \]  \hspace{1cm} (13)
\[ \frac{1}{y} \frac{dy}{dx} = a \frac{n x^{n-1}}{x^n} \]  \hspace{1cm} (14)
\[ \frac{1}{y} \frac{dy}{dx} = \frac{n}{x} \]  \hspace{1cm} (15)
\[ \frac{dy}{y} = n \frac{dx}{x} \]  \hspace{1cm} (16)
\[ n = \frac{dy}{y} \frac{dx}{x} \]  \hspace{1cm} (17)

The variable n essentially represents the relative change in y over the relative change in x.

Similarly we can show that n is linear in logarithmic space by Equation 18-20,

\[ y = ax^n \]  \hspace{1cm} (18)
This derivation shows how the normalized sensitivity coefficient becomes analogous to the slope of the function in logarithmic space.

More generally, consider the function (Equation 21):

\[ y = f(x_1, x_2, x_3, x_4), \]  

which is analogous to the SEF, where \( y = \ln[\text{OH}] \) and \( x_n = \ln[J(\text{NO}_2)], \ln[H_2O], \ln[\text{VOCs}], \) and \( \ln[\text{NO}_x] \), respectively. Using a Taylor series expansion (Equation 22) and only keeping the first ordered terms:

\[ y \approx y_0 + \frac{\partial f}{\partial x_1} x_1 + \frac{\partial f}{\partial x_2} x_2 + \frac{\partial f}{\partial x_3} x_3 + \frac{\partial f}{\partial x_4} x_4 \]  

\[ \alpha = \frac{\partial y}{\partial x_1}, \beta = \frac{\partial y}{\partial x_2}, \text{ etc.} \]  

Equation 23 shows that the normalized sensitivity coefficients (\( \alpha, \beta, \gamma, \delta \)) represent the relative change in the short-lived quantity \( y = \ln[\text{OH}] \) over the relative change in the individual photochemical drivers \( x_n = \ln[J(\text{NO}_2)], \ln[H_2O], \ln[\text{NO}_x], \) and \( \ln[\text{VOCs}] \). Taking the exponent on both sides of the equation we get Equation 24,

\[ e^y \approx e^{y_0 + \alpha x_1 + \beta x_2 + \gamma x_3 + \delta x_4} \]  

and substituting \( y = \ln[\text{OH}] \) and the other terms gives equation 10:

\[ [\text{OH}] = A [J(\text{NO}_2)]^\alpha [H_2O]^\beta [\text{NO}_x]^\gamma [\text{VOCs}]^\delta \]  

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d. Box model calculation of normalized sensitivity coefficients

The box model used in this study to recover the sensitivity coefficients was the NCAR Master Mechanism (Madronich and Calvert, 1990) box model. This gas phase chemistry model involves approximately 2000 chemical reactions with ~5000 species. The box model follows a parcel along its path without deposition or any additional emissions. The initial chemical conditions used can be found in Table 3.

Table 3. Initial chemical conditions used in box model*

<table>
<thead>
<tr>
<th>Species</th>
<th>Mixing ratio (ppbv)</th>
<th>Species</th>
<th>Mixing ratio (ppv)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₃</td>
<td>30</td>
<td>Ethene</td>
<td>22</td>
</tr>
<tr>
<td>NO</td>
<td>80</td>
<td>Propane</td>
<td>5</td>
</tr>
<tr>
<td>CO</td>
<td>3000</td>
<td>1-Butene</td>
<td>2.9</td>
</tr>
<tr>
<td>Methane</td>
<td>26000</td>
<td>2-Butene</td>
<td>2.7</td>
</tr>
<tr>
<td>Ethane</td>
<td>14</td>
<td>i-Butene</td>
<td>1.8</td>
</tr>
<tr>
<td>Propane</td>
<td>160</td>
<td>Ethyne</td>
<td>3.2</td>
</tr>
<tr>
<td>n-Butane</td>
<td>70</td>
<td>Isoprene</td>
<td>0.52</td>
</tr>
<tr>
<td>i-Butane</td>
<td>33</td>
<td>Benzene</td>
<td>4.6</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>14</td>
<td>Toluene</td>
<td>21</td>
</tr>
<tr>
<td>i-Pentane</td>
<td>19</td>
<td>Xylenes</td>
<td>10</td>
</tr>
<tr>
<td>Hexanes</td>
<td>28</td>
<td>CH₂O</td>
<td>23.9</td>
</tr>
</tbody>
</table>

*Table modified from Madronich, 2006

Other conditions were applied, e.g., NOₓ values were set to 140 ppb, hydrocarbons were set to 1500 ppbC and the temperature was set at 283 K. The chemistry was allowed to dilute with background air and the sensitivity coefficients were chosen for day 2.5. Dilution after 2.5 days was chosen because it is representative of our desired remote conditions. The final sensitivity coefficients used can be seen in Table 4.

Table 4. Box Model Sensitivity Coefficients for OH (x100)

<table>
<thead>
<tr>
<th>Individual driver</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>J(NO₂)</td>
<td>100</td>
</tr>
<tr>
<td>H₂O</td>
<td>30</td>
</tr>
<tr>
<td>NOₓ</td>
<td>700</td>
</tr>
<tr>
<td>VOCs</td>
<td>-100</td>
</tr>
</tbody>
</table>

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3. Results and Discussion

a. Single Parameter Correlations

To solidify the fact that OH does not contain one absolute dominant driver, we correlated the OH concentration retrieved from the WRF/Chem simulation with each individual driver. It can be seen from Figure 2 that the correlations were poor and contained much scatter.

Fig. 2. OH concentration in molecules/cm$^3$ provided by WRF/chem model correlated with each individual driver used in semi-empirical function. a) J(NO$_2$) plot with correlation coefficient of 0.67 b) H$_2$O plot with correlation coefficient of 0.22 c) NO$_x$ with a correlation of 0.11 d) VOCs with a correlation of -0.23.
b. **Multiple parameter correlations**

In order to balance the effect of all the dominant drivers, we use the semi-empirical function with each driver containing their respective sensitivity coefficient. When the SEF was applied, we saw much improved correlation, with a correlation coefficient of 0.73. The SEF could explain 53% of the variance. Although the correlation improved with comparison to the individual drivers, the data showed multiple correlation lines, as seen in Figure 3.

![Figure 3](image.png)

**Fig. 3.** OH concentration correlated with the semi-empirical function. Data has a correlation coefficient of 0.73 and a slope of $6.372 \times 10^{-4}$.

This “fork” was seen in most of the days available in the data; some days had a clearer signal than others, but the multiple lines continued to appear. Different times were explored as well and this characteristic was still prominent.

c. **Comparing VOCs with CO in SEF**

One possible explanation for the “fork” in the data is due to a possible issue in how the different chemical mechanisms calculate the VOC reactivity rates with OH and also the way they are lumped together. In order to remove any biases with VOCs, we removed them from the weighted sum and only used the CO concentration, using the VOC sensitivity coefficient, as seen in Figure 4.
Fig. 4. OH concentration correlated with the semi-empirical formula, but using CO concentration only for the VOCs. Multiple lines are still seen in data. Correlation coefficient for data is 0.50 with a slope of $1.47 \times 10^9$ molecules cm$^{-3}$ sec$^{-1}$.

Using the same conditions as before, we observed the same “fork” in the data. This showed that there was not a strong sensitivity to VOCs as previously hypothesized. Although removing VOCs did not explain the multiple correlations lines, it was observed that the inclusion of VOCs did in fact improve the correlation, from 0.50 to 0.73, and reduced the variance. It seems that VOCs dominate the OH concentration enough to explain 28% more of the variance than just using the concentration of CO.

d. Boundary sensitivity

We had the suspicion that the multiple lines might be due to differences in the chemistry at the modeling domain boundaries; and so the West and South boundaries were cropped by 504 km and the North and East boundaries were cropped by 240 km. This in fact, reduced the variance and eliminated one of the two correlation lines observed in Figure 3. The correlation coefficient improved from 0.73 to 0.86 as seen in Figure 5.
Fig. 5. OH concentration correlated with SEF. Data near boundaries was cropped out, 504 km from the West and South boundaries and 240 km from the North and East boundaries. Data contains a slope of $4.951 \times 10^{-4}$ correlation coefficient of 0.86 and so after cropping the boundaries of the domain, the SEF explains approximately 74% of the variance.

Cropping the domain boundaries removed the bias from the inconsistencies in the two chemical mechanisms, CBM-Z and MOZART. It seems that MOZART and CBM-Z calculate OH concentrations differently. This is a concern because if the line of data that was removed belonged to MOZART, the mechanism would have calculated twice as much OH than CBM-Z for the same SEF value. That makes a large impact when computing the lifetime of greenhouse gases like methane and carbon dioxide.

e. Comparing chemical mechanisms

The linear relationship observed after cropping the boundaries was for data using CBM-Z. WRF/Chem has the option of using either CBM-Z or SAPRC for the chemical mechanism. Although they have slight differences, they should perform the same general chemistry and thus, both contain the linearity seen in Figure 5. Comparing both CBM-Z and SAPRC, in figure 6, for the same conditions and removing the VOCs to avoid any difference in reactivity calculations, we do in fact see the linear relationship.
Fig. 6. OH concentration correlated against the SEF but only with CO concentration for VOCs. a) This is the plot using the CBM-Z chemical mechanism. Data contains a correlation coefficient of 0.57 with a slope of $1.125 \times 10^9$ molecules cm$^{-3}$ sec$^{-1}$. b) This is the plot using the SAPRC chemical mechanism. Data contains a correlation coefficient of 0.78 and a slope of $2.687 \times 10^9$ molecules cm$^{-3}$ sec$^{-1}$.

An interesting observation was seen in the linear regression line slopes of both chemical mechanisms. The slope for SAPRC was twice as steep compared to that of CBM-Z, which means that SAPRC is predicting twice as much OH as CBM-Z. Including the VOCs, the linearity was still seen in both mechanisms (Figure 7). The SAPRC slope was still approximately twice as steep as the CBM-Z slope.

Fig. 7. Similar to Figure 6, but these plots contain the reactivity-weighted sum of VOCs. Data still shows relatively linear relationship and due to the addition of the VOCs, the correlation improved. a) Plot using CBM-Z contains correlation coefficient 0.74 with a slope of $4.74 \times 10^{-4}$ b) Plot using SAPRC contains correlation coefficient of 0.81 with a slope of $7.724 \times 10^{-4}$.
f. Comparing model outputs with observations

To evaluate the WRF/Chem model simulation for the MIRAGE field campaign, we compare the measurements taken during MIRAGE with the model output. In Figure 8, the two plots can be seen. Similar conditions from Table 2 were used for both cases and it was observed that the correlation coefficient for the measurements was larger than that for the model output. The SEF can explain 66% of the variance in the measurements and this is without including the VOC reactivity-weighted sum.

![Fig. 8. OH concentration correlated with the SEF with CO concentrations for the VOCs.](image)

Although the correlation for measurements was better than for model output, it seems that there are still issues with the model data. Figure 8.a seems to contain branches of data. When the exact linear regression line is placed on to the model output plot, it is observed to lie in the center region of points were the primary line of the data seems to be. If the outside branches of the center region can be explain and the correlation line can be tightened, that would mean that the model simulation would have successfully simulated the OH concentration seen in the MIRAGE measurements.
4. Conclusion and Future Work

Single parameter correlations do not provide a full explanation of the variance, but when the SEF is applied there is a great improvement in the correlation. This relationship had to be further explored due to the observations of multiple correlation lines. There is not a strong sensitivity to VOCs but when using the reactivity-weighted sum we observe the correlation lines to tighten and improve.

The multiple lines observed may be due to the different chemical mechanisms and boundary conditions, but this is an area that needs to be further studied. A direct comparison between MOZART and CBM-Z needs to be performed to explore and understand the differences in the mechanisms. More research needs to be done to further compare CBM-Z to SAPRC to understand why SAPRC contains a slope twice as steep as CBM-Z. In addition to the slope, more research needs to be conducted to understand how VOC reactivities are calculated in each chemical mechanism. To compare the two mechanisms, the VOCs must be summed up in an equivalent way.

This study began to look into model versus measurements, but it was only at a basic level. The next step would be to include the VOCs for both model and measurements. The challenge in that would be retrieving the VOC reactivities with respect to OH. These rates may be calculated differently in the measurements than in the model.

Further questions would have to be explored, i.e., do aerosols matter? How would we take aerosols into account when working with this method? Due to time constraints, this study was only able to explore OH concentrations, but would this method work for other short-lived radicals such as HO₂ and NO/NO₂? If other radicals were to be studied, their sensitivity coefficients would have to be calculated. This study used sensitivity coefficients for remote
conditions, but this method could also be expanded to different chemical regimes, i.e., urban conditions.

We found many interesting observations throughout this study, but no definite conclusions. There is still much more that needs to be explored and due to limited time, we were not able to continue the research. This method may become a powerful test for evaluating the fast photochemistry of three-dimensional models and measurements in the future.

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