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## **FINAL REPORT**

### **AQRP Project 22 - 003**

# **Evaluating the Ability of Statistical and Photochemical Models to Capture the Impacts of Biomass Burning Smoke on Urban Air Quality in Texas**

Revision 2.0

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### **List of Acronyms**

CAMx – Community Atmosphere Model with Extensions

ELP – El Paso

EPA – Environmental Protection Agency

GAM – Generalized Additive Model

HGB – Houston-Galveston-Brazoria

MDA8 – Maximum Daily 8-hour Average

QAPP – Quality Assurance Project Plan

STILT – Stochastic Time-Inverted Lagrangian Transport

TCEQ – Texas Commission on Environmental Quality

WRF – Weather Research and Forecasting Model

## Executive Summary

The objectives of this project were to:

- (1) Use generalized additive models (GAMs) driven with satellite and surface observations to examine the impact of fires on background and total O<sub>3</sub> and PM<sub>2.5</sub> in Texas urban areas.
- (2) Examine the ability of CAMx photochemical model to simulate these fire impacts by applying similar statistical methods to the CAMx results.
- (3) Use any statistically significant differences found to prioritize different approaches to improve the ability of CAMx to simulate the impacts of domestic fires on air quality.

We performed a statistical analysis using generalized additive models (GAMs) to see how fires impacted background and maximum concentrations of O<sub>3</sub> and PM<sub>2.5</sub> in Houston and El Paso. Our results suggest that on days when the HMS indicated smoke over Houston and El Paso, the daily average PM<sub>2.5</sub> was elevated by 1.4-2.6 µg/m<sup>3</sup> on average (background and maximum) while the background MDA8 O<sub>3</sub> was elevated by 2.4-8 ppbv on average. Unfortunately, the results depend strongly on which set of fire predictors is used. For Houston, the change in O<sub>3</sub> impact as the smoke enters the city varies from -0.9 ppbv to +6.0 ppbv, with three out of four methods predicting an increase in mean O<sub>3</sub> as the smoke enters the city. In El Paso, the change in mean O<sub>3</sub> impact as the smoke enters the city varies from -1.6 ppbv to -0.5 ppbv. The geographic fire variables from Sec. 4.1.3 give the best fitting statistics and predicts fire impacts of 7.0-8.0 ppbv in both urban areas, with a slight decrease in the impact when the smoke enters the city.

We also performed a statistical analysis using generalized additive models (GAMs) to see if the CAMx predictions were consistent with the impact of fires on background and maximum concentrations of O<sub>3</sub> in Houston and El Paso. For El Paso, our analysis suggested that there were statistically significant differences between CAMx and the ambient data, but further analysis showed that the predicted impacts of fires in both cases were very similar. For Houston, however, the differences between CAMx and the ambient data fits were not statistically significant for maximum O<sub>3</sub>, but the CAMx data strongly overestimates the background O<sub>3</sub> for Houston on both smoky and non-smoky days.

Since CAMx generally appears to give similar predictions for the impacts of smoke as the ambient data, there is little need to identify areas for improvement as called for in Objective 3 of this project. The exception is for the impacts of smoke on Houston background O<sub>3</sub>, where CAMx predicts a 2 ppb larger impact. This is likely related to the general large overestimate of background O<sub>3</sub> by CAMx in Houston but may also be due to errors in the chemistry as emissions from the Yucatan interact with halogens over the Gulf.

In addition, our results showed that CAMx overestimates Houston background O<sub>3</sub> on both smoky and non-smoky days, suggesting that further work needs to be done on ozone-destroying halogen emissions and chemistry and on the biogenic emissions upwind of Houston. Similarly, the underpredictions of maximum O<sub>3</sub> in El Paso suggest that further work is needed on CAMx emissions for El Paso and Ciudad Juarez and the O<sub>3</sub> chemistry within the combined urban area.



Future work should focus on finding ways to better determine the best set of smoke predictors for use in statistical studies such as this, with a focus on high tail events where smoke could lead to an exceedance of air quality standards using methods from Brown-Steiner et al. (2021). While the predictions of smoke impact on  $O_3$  from CAMx appear to be reasonable based on this study, our results suggest that further work is needed to (a) address the overestimate of Houston background  $O_3$  on both smoky and non-smoky days and (b) the underpredictions of maximum  $O_3$  in El Paso.

## 1 Introduction

Understanding the impact of domestic fire smoke on urban air quality (AQ) requires understanding (i) the chemistry of the smoke before it reaches the city and (ii) the changes in the urban production rate of  $O_3$  and  $PM_{2.5}$  caused by the smoke. The relative importance of these two pathways on the air quality impacts of domestic fire smoke is not well understood and it is unclear which processes should be targeted to reduce the overall uncertainty.

In addition, three-dimensional (3D) photochemical models like CAMx can have trouble representing the near-source chemistry of the smoke plume and the impact of smoke mixing with urban pollution due to a combination of low spatial resolution near fires and incorrect representation of the chemistry of smoke-specific VOCs (e.g., Baker et al., 2016). These limitations in physical approaches have led to the development of a variety of statistical approaches to estimate the impact of biomass burning on urban AQ (e.g., Gong et al., 2017; de Foy et al., 2021). However, little work has been done to compare the statistical and 3D photochemical approaches or to identify priorities for further development of both approaches. Thus, the US EPA and US Forest Service organized assessment of smoke research needs noted this was a key priority for future smoke chemistry research (Alvarado et al., 2022).

Thus, the objectives of this project are to:

- (1) Use generalized additive models (GAMs) driven with satellite and surface observations to examine the impact of fires on background and total  $O_3$  and  $PM_{2.5}$  in Texas urban areas.
- (2) Examine the ability of CAMx photochemical model to simulate these fire impacts by applying similar statistical methods to the CAMx results.
- (3) Use any statistically significant differences found to prioritize different approaches to improve the ability of CAMx to simulate the impacts of domestic fires on air quality.

In this final report, we examine the impact of fires on urban AQ in Texas using statistical modeling (Objective 1) and the ability of CAMx photochemical model to simulate these fire impacts by applying similar statistical methods to the CAMx results (Objective 2). Two urban areas were examined: Houston-Galveston-Brazoria (HGB) and El Paso. Background  $O_3$  and  $PM_{2.5}$  concentrations were estimated using the lowest value observed at sites near the border of the area of interest, as TCEQ has done in the past (e.g., Berlin et al., 2013). Analyzing the impacts of fires on background and urban sites separately allows us to examine the change in  $O_3$  and  $PM_{2.5}$  due to the mixing of smoke with urban pollution separately from the impact of smoke before it mixes with urban pollution.

Below we discuss the dataset for this project, including the smoke and fire predictors developed so far for this project (Section 2), the statistical modeling approach (Section 3), and our initial findings (Section 4). Section 5 discusses our QA findings, Section 6 summarizes our conclusions, and Section 7 describes our plans for future research.

## 2 Dataset for Model Training

### 2.1 Ambient Air Quality Data

Maximum daily 8-hour average (MDA8) O<sub>3</sub> mixing ratios and daily average PM<sub>2.5</sub> concentrations will be calculated for each HGB and El Paso site from the surface air quality data in TAMIS. Sites in each urban area were separated into background (for sites on the outskirts of the city) and urban (for sites near the city core). For each urban area, the minimum value of MDA8 O<sub>3</sub> and daily average PM<sub>2.5</sub> from background sites upwind of the urban core were selected as the background estimate for that day, while the maximum concentrations were selected as the urban maximum.

### 2.2 Meteorological Predictors

The meteorological predictors to be used in this study (Table 1) are based on our previous GAM studies of the ability of meteorological predictors to estimate the concentrations of O<sub>3</sub> and PM<sub>2.5</sub> at urban and background monitoring sites in Texas. Our team has shown that these meteorological predictors, plus the previous day's MDA8 O<sub>3</sub> or daily average PM<sub>2.5</sub>, can explain approximately 70% of the variability in background and urban O<sub>3</sub>, and about 30-40% of the variability in background and urban PM<sub>2.5</sub> (e.g., Alvarado et al., 2015; McVey et al., 2018; Pernak et al., 2019; Brown-Steiner et al., 2021).

Table 1. Meteorological parameters used in the GAMs. The column name is given in italics.

|  |
|--|
| 1) Afternoon mean temperature (°C, <i>afternoon_mean_T, 1-4 PM CST</i> )   |
| 2) Diurnal temperature change (°C, <i>diurnal_T</i> )  |
| 3) Daily average wind speed (m/s, <i>daily_ws</i> )  |
| 4) Daily average wind direction (degrees clockwise from North, <i>daily_wd</i> )   |
| 5) Daily average water vapor density (g/m <sup>3</sup> , <i>SWVP</i> )   |
| 6) Morning surface temperature difference (1200 UTC) (temperature at 925 or 700 mb–temperature at surface at 1200 UTC) (°C, <i>T_dif_925mb</i> or <i>T_dif_700mb</i> ) |
| 7) Transport direction (degrees clockwise from North, <i>HYSPLIT_Bearing</i> )   |
| 8) Transport distance (m, <i>HYSPLIT_dist</i> )  |

Variables 1-5 in Table 1 were calculated from the surface meteorological data in the Texas Air Monitoring Information System (TAMIS). Variable 6, which reflects the vertical stability of the atmosphere each day, was calculated from upper atmosphere data in the Integrated Global Radiosonde Archive (IGRA Version 2). Given El Paso's higher elevation, an upper atmosphere level of 700 mbar was used for this city as opposed to the 925 mbar value used for all other urban areas. Variables 7 and 8 were calculated from 24-hour NOAA Hybrid Single-Particle Lagrangian Integrated Trajectory model (HYSPLIT) back-trajectories driven with 12 km horizontal resolution NAM data. As in Camalier et al. (2007), these back-trajectories are calculated assuming an initial height of 300 m above ground level (AGL) and are started at noon local solar time. The endpoints of the back-trajectories were used to calculate the 24-hour transport direction and distance for each urban area for the 2012-2021 period.

### 2.3 Fire and Smoke Predictors

The NOAA Hazard Mapping System (HMS) Fire and Smoke product will be our primary source of fire predictors, as we have shown that days where the HMS product indicates smoke over Houston tend to be associated with enhancements in CO, O<sub>3</sub>, NO<sub>x</sub>, and NO<sub>y</sub> (Figure 1). This gives us confidence in the ability of our statistical modeling to be able to identify a statistically significant impact of fires on air quality in HGB and El Paso. To make the HMS, satellite analysts compare automated fire detections to the infrared satellite images used to produce them to ensure each fire exists (Ruminski et al., 2006; Schroeder et al., 2008; Brey et al., 2018). Small fires are more difficult to detect and are underreported (*e.g.*, Hu et al., 2016). False fire detections are removed, and fires that were not automatically detected are added manually.

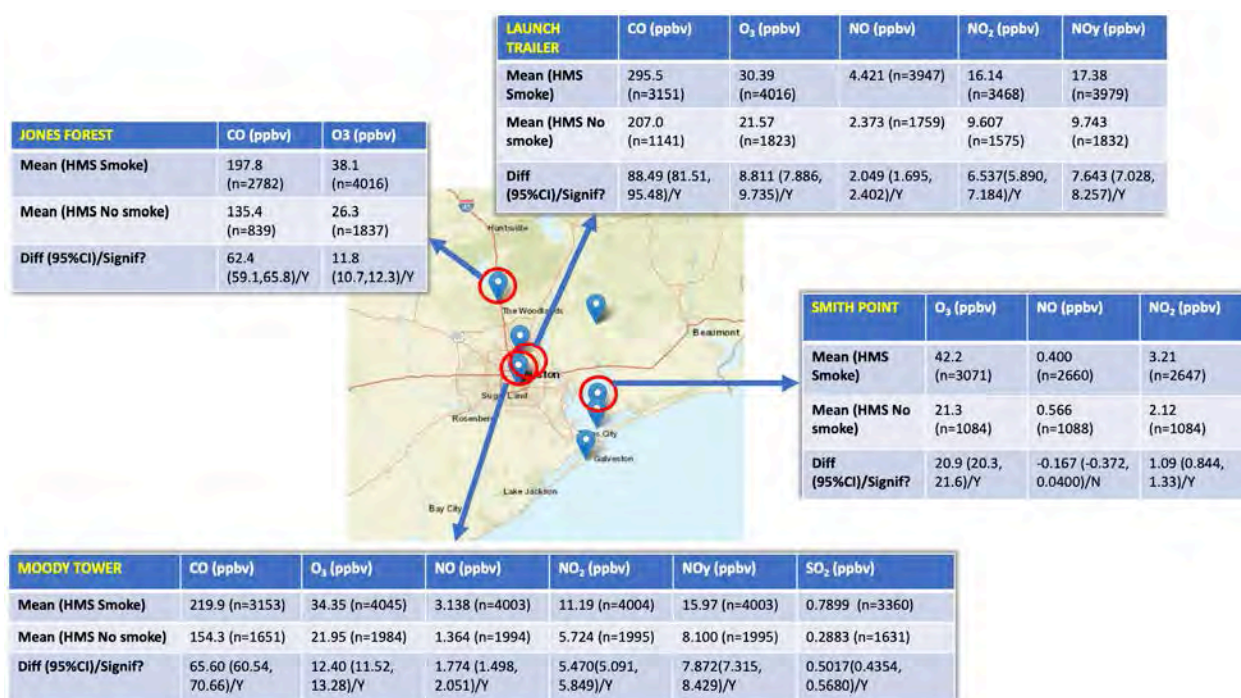


Figure 1. Map of selected surface air quality monitoring sites in HGB. Tables show concentrations of species measured at each circled site, divided into HMS-smoke and HMS-no smoke categories.

After identifying fire locations, HMS analysts use imagery from multiple NOAA and NASA satellites to identify the geographic extent of smoke plumes (Rolph et al., 2009; Ruminski et al., 2006). Due to the frequent interference by cloud cover, the number and extent of smoke plumes reported in the HMS represents a conservative estimate.

In addition to the HMS, we use the Fire Inventory from NCAR (FINN v2.5, Wiedinmyer et al., 2011, McDonald-Buller et al., 2015) to determine fire counts within different distances from the city center (0.5, 1.0, 2.5, 5.0, 10.0, and 25.0 degrees (lat/lon) from the city).

We also convolved the FINN 0.1-degree estimates of total NO<sub>x</sub>, volatile organic compounds (VOC), and PM<sub>2.5</sub> emissions from fires with daily estimates of upwind influences on HGB and El Paso measurements (i.e., upwind surface “footprints” calculated from STILT) to determine the daily transport of O<sub>3</sub> precursors and primary PM<sub>2.5</sub> to each city. The Stochastic Time-Inverted Lagrangian Transport (STILT) model (Lin et al., 2003; Nehr Korn et al., 2010) is an enhanced version of the HYSPLIT model (Draxler and Hess, 1998) aimed at mass conservation, a critical consideration for inversion work. STILT computes the “footprint” (adjoint of the transport field) by following an ensemble of tracer particles backwards in time from the location of each measurement (“receptor”). The footprint (units: ppm/μmol m<sup>-2</sup> s<sup>-1</sup>) quantifies the concentration enhancement at the receptor at each point in time due to unit surface flux at each upwind location. Here we will generate daily STILT footprints for each urban area driven with 12 km NAM meteorological data. As with the HYSPLIT predictors in Section 1.2.1.2, these footprints will be initialized at local noon at a height of 300 m and will go at least 72 hours back in time.

Note that, as STILT does not account for the chemistry along the transport path, it cannot directly account for the chemical formation of O<sub>3</sub> and PM<sub>2.5</sub> as the smoke is transported from the fire. Instead, we will use the STILT footprints multiplied by the FINN fire emissions as an indicator of smoke transport and see how this smoke indicator correlates with O<sub>3</sub> and PM<sub>2.5</sub>. We will also examine how the predictions depend on smoke age by segregating the footprint predictors into fresh smoke (< 24 hours transport time from fire to city) and aged smoke (≥ 24 hours).

Here we test several fire and smoke predictors based on the HMS and FINN data, including:

- a. A binary predictor for the presence of smoke according to the NOAA HMS (Figure 1)
- b. The total FINN fire counts in surrounding regions binned by distance from the city at 0.5, 1.0, 2.5, 5.0, 10.0, and 25.0 degrees (lat/lon).
- c. FINN fire counts and total emissions for different geographic regions: Yucatan, all of Mexico, California, and states bordering Texas (LA, AR, OK, NM).
- d. WRF-STILT footprints for NO, NO<sub>2</sub>, CO<sub>2</sub>, and CO.

## 2.4 CAMx Data

TCEQ generated CAMx output for the Houston (4 km horizontal resolution) and El Paso (12 km resolution) for the year 2019 was used for the comparison with observed data. MDA8 O<sub>3</sub> values were calculated for each monitoring location based on the CAMx grid box that contained the monitoring location. New CAMx-based values for the maximum MDA8 O<sub>3</sub> and background MDA8 O<sub>3</sub> value for each urban area by date were calculated using the same methods used for the ambient data (Section 2.1). These were added to the model training dataset with a new flag, “Is\_Model”, which is 1 for data from CAMx and 0 for ambient data. All other parameters were kept identical for the “Is\_Model” cases, such that the new lines only differ from the ambient data in their values for Max MDA8 O<sub>3</sub>, background MDA8 O<sub>3</sub>, and Is\_Model.

## 3 Generalized Additive Models

GAMs are a form of linear modeling which allows non-linear functions of individual predictors within a regression framework (Wood, 2017). This is like standard linear regression techniques, which optimize scalar coefficients ( $\alpha_k$ ) for each predictor ( $x_k$ ) for  $k = 1$  to  $p$ :

$$\hat{y} = \alpha_0 + \alpha_1 x_1 + \alpha_2 x_2 + \dots + \alpha_p x_p$$

except that the coefficients are replaced with potentially non-linear smooth functions:

$$\hat{y} = s_0 + s_1(x_1) + s_2(x_2) + \dots + s_p(x_p)$$

The GAM approach optimizes these smooth functions. An advantage of GAMs over neural networks and similar machine learning techniques is that it is easy to isolate the effects of the individual variables in GAMs. This will allow us to separate the impact of fire-related variables from the impact of the rest of the predictors. A potential disadvantage relative to standard linear regression is that the smooth functions can overfit the data, and so care needs to be taken to ensure that the derived smooth functions are realistic and robust to changes in the training data set. To address this, the R package *mgcv* includes routines to fit GAMs, examine the models graphically, and test their robustness via k-fold cross-validation and other techniques.

In this study, all meteorological predictors and the FINN fire counts were simulated as smooth functions using cubic spline basis set, with periodic splines used to account for the effects of the day of year and HYSPLIT bearing. Year, day of week, and the HMS smoke flag were included as factor variables. The models predict the natural logarithm of O<sub>3</sub> and PM<sub>2.5</sub> concentrations as these are usually log-normally distributed.

## 4 Results

### 4.1 Objective 1: Impact of fires on urban AQ in Texas

#### 4.1.1 Smoke Flag Tests

In these tests, we trained GAMs by adding the HMS smoke flag to the meteorological predictors listed in Section 2.2. For ozone, the HMS smoke flag was always a significant predictor ( $p < 0.001$ ). All predictors included were highly significant ( $p < 0.001$ ) in Houston, while in El Paso they were all highly significant except for afternoon mean temperature, which was still very significant ( $p < 0.02$ ). Table 2 summarizes the change in the quality of the model fits with and without the smoke flags by examining the deviance explained, the total model degrees of freedom, and the Akaike information criterion (AIC). A lower AIC indicates a better model fit. In all cases, adding the HMS smoke flag leads to a slightly better model fit while the increase in degrees of freedom for the model is less than 1.

Table 2. Degrees of freedom (df), Akaike information criterion (AIC), and deviance explained (Dev. Exp., %) for each ozone model.

|               | With Smoke Flag |       |           | Without Smoke Flag |       |           |
|---------------|-----------------|-------|-----------|--------------------|-------|-----------|
|               | df              | AIC   | Dev. Exp. | df                 | AIC   | Dev. Exp. |
| Houston Bkgrd | 46.9            | 16353 | 63.7%     | 46.2               | 16445 | 63.4%     |
| Houston Max   | 46.5            | 17129 | 67.2%     | 45.9               | 17224 | 67.0%     |
| El Paso Bkgrd | 44.2            | 15350 | 51.5%     | 43.4               | 15429 | 51.0%     |
| El Paso Max   | 43.1            | 15696 | 54.2%     | 42.2               | 15764 | 53.9%     |

With these models, we then estimate the impact of smoke on background and maximum MDA8 O<sub>3</sub> in each urban area by calculating the GAM predictions with the true smoke flag minus the GAM predictions when the smoke flag is set to 0 for all days. We calculated this difference for all days where the HMS indicated smoke over the city (~10% of days). The distributions of these smoke-related differences are summarized in Table 3. We see similar mean impacts on background MDA8 O<sub>3</sub> in each urban area (2.4 ppbv). However, in Houston we see a slight increase in MDA8 O<sub>3</sub> (0.2 ppbv) in the city on smoky days, while in El Paso we see a slight decrease (0.5 ppbv). This suggests that in city chemistry has little impact on the ozone impacts from smoke and can either increase or decrease those impacts. Note that while these tests only account for the presence of smoke as indicated by HMS, not its concentration, we can conclude that the presence of smoke over the city as indicated by HMS is associated with an increase in MDA8 O<sub>3</sub> that can vary from 1.2 ppbv to 4.8 ppbv, and thus the HMS smoke product can be treated as significant evidence that the MDA8 O<sub>3</sub> for a given day was increased by smoke.

Table 3. Change in MDA8 O<sub>3</sub> due to the presence of smoke as indicated by the HMS smoke flag in the GAMs trained only on the meteorological predictors and the HMS smoke flag.

|                             | <b>Houston MDA8 O<sub>3</sub></b> |            | <b>El Paso MDA8 O<sub>3</sub></b> |            |
|-----------------------------|-----------------------------------|------------|-----------------------------------|------------|
|                             | Bkgrd (ppbv)                      | Max (ppbv) | Bkgrd (ppbv)                      | Max (ppbv) |
| Minimum                     | 1.2                               | 1.5        | 1.7                               | 1.4        |
| 25 <sup>th</sup> Percentile | 1.9                               | 2.1        | 2.2                               | 1.8        |
| Median                      | 2.3                               | 2.5        | 2.4                               | 1.9        |
| Mean                        | 2.4                               | 2.6        | 2.4                               | 1.9        |
| 75 <sup>th</sup> percentile | 2.8                               | 3.0        | 2.5                               | 2.0        |
| Max                         | 4.7                               | 4.8        | 2.9                               | 2.4        |
| Std. Dev.                   | 0.64                              | 0.60       | 0.23                              | 0.19       |

Unfortunately, the PM<sub>2.5</sub> GAM fits, both with and without the smoke flag, showed very poor performance. The total deviance explained generally less than 30%, and the residual plots versus fitted values (not shown) indicated significant heteroskedacity in the data. Several variable transformations were attempted to resolve this issue, but not removed the heteroskedacity. Simple correlation analysis also suggested that further attempts were unlikely to succeed, as the predictor variables have very low correlations with either background or maximum PM<sub>2.5</sub>.



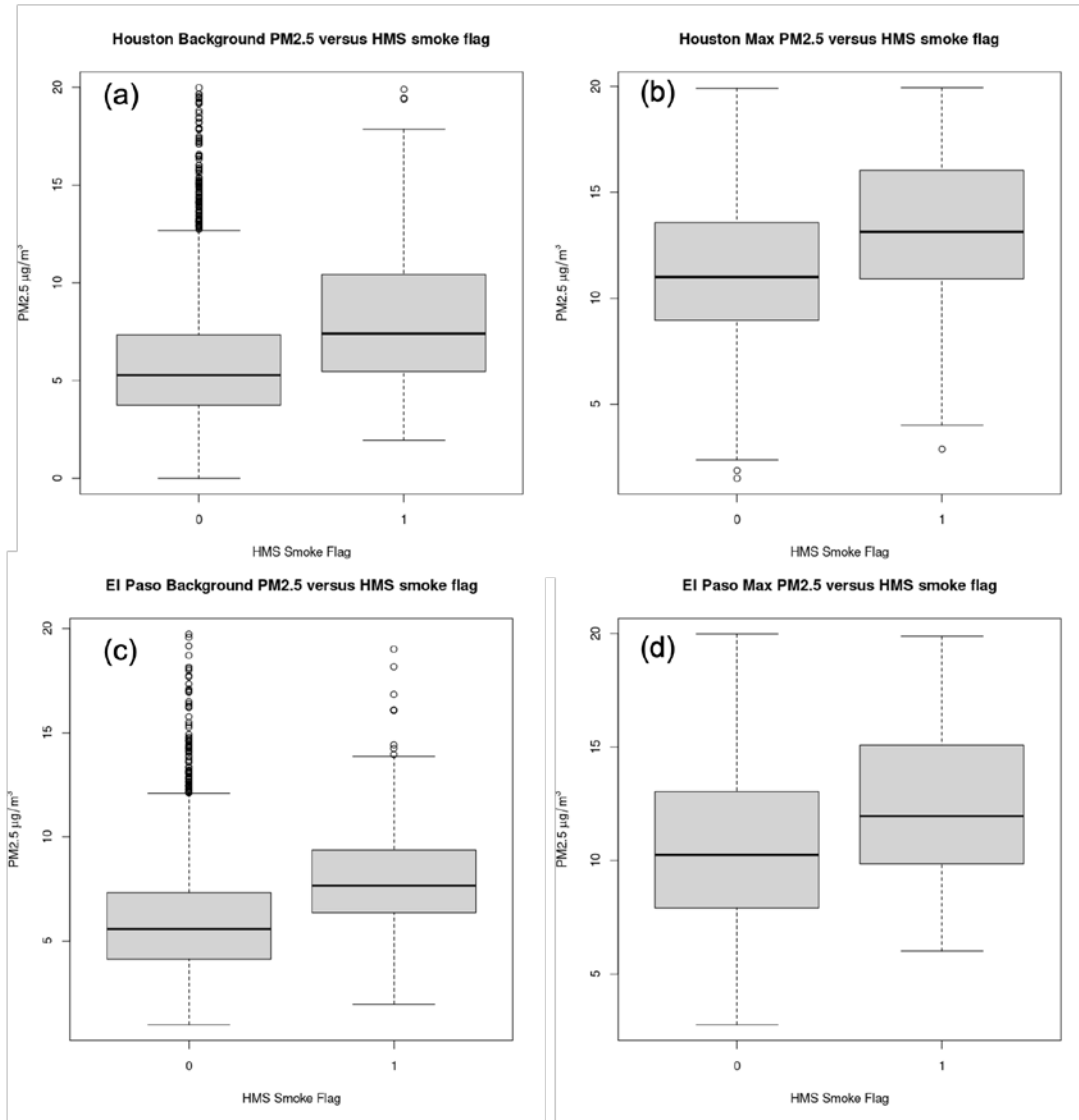


Figure 2. Box and whisker plots of the daily average  $PM_{2.5}$  differences on days with the HMS indicating smoke overhead (smoke flag = 1) and with no smoke overhead (smoke flag = 0). (a) Houston background  $PM_{2.5}$ . (b) Houston maximum  $PM_{2.5}$ . (c) El Paso background  $PM_{2.5}$ . (d) El Paso Maximum  $PM_{2.5}$ .

Thus, instead of showing GAM fit results that are unreliable, we used the simpler approach of comparing the distributions of maximum and background  $PM_{2.5}$  for days with and without HMS smoke. Figure 2 shows box plots for the four cases. In all cases, the  $PM_{2.5}$  distributions on days where HMS indicated smoke have higher mean  $PM_{2.5}$  concentration, and the differences in the means (t-test) and the distributions (Kolmogorov-Smirnov test) are statistically significant at  $p < 0.001$ . The 95% confidence intervals of the mean differences are:

- Houston  $PM_{2.5}$  Background: 1.9-2.6  $\mu\text{g}/\text{m}^3$
- Houston  $PM_{2.5}$  Max: 1.5-2.3  $\mu\text{g}/\text{m}^3$
- El Paso  $PM_{2.5}$  Background: 1.7-2.5  $\mu\text{g}/\text{m}^3$
- El Paso  $PM_{2.5}$  Max: 1.5-2.6  $\mu\text{g}/\text{m}^3$

This suggests that on average, days where the HMS indicated smoke overhead have about  $2 \mu\text{g}/\text{m}^3$  more  $\text{PM}_{2.5}$  at the surface, but that these differences do not significantly change between the background and the city core, so the urban chemistry has little impact on the  $\text{PM}_{2.5}$  impact of fires.

#### 4.1.2 FINN fire count tests

We then added the different FINN fire count bins to our  $\text{O}_3$  GAMs without the HMS smoke flag to determine which count distance improved the fit the most. The different predictors were evaluated using the deviance explained by the GAM, the minimized generalized cross-validation (GCV) score, and the statistical significance of the predictor in the fit. The results for background  $\text{O}_3$  are shown in Table 4 and the results for maximum  $\text{O}_3$  are in Table 5. For El Paso, the best results are for using a  $\pm 25$  degree (lat/lon) box around the city to calculate fire counts. This area includes the Yucatan peninsula and California, major locations of annual fires. The Houston maximum  $\text{O}_3$  is best fit with a  $\pm 10$ -degrees box, which includes the Yucatan. For Houston background  $\text{O}_3$ , the  $\pm 5$ -degree box is slightly better, but to keep consistency with the maximum we choose to use the 10-degree box. In all cases, adding the smoke flag to the chosen FINN fire count predictor increases the quality of the fit. Thus, we examine the fire impacts on ozone implied by the GAMs using (a) the meteorological predictors from Section 2.2, (b) the HMS smoke flag, and (c) the FINN fires counts at  $\pm 10$ -degrees from Houston and  $\pm 25$ -degrees from El Paso. This suggests that the impact of smoke is primarily from remote fires (1000 to 2500 km away).

Table 4. Quality of fit for GAMs using different FINN fire count predictors to predict maximum MDA8  $\text{O}_3$ .

|                       | Houston Max MDA8 $\text{O}_3$ |               |                  | El Paso Max MDA8 $\text{O}_3$ |               |                  |
|-----------------------|-------------------------------|---------------|------------------|-------------------------------|---------------|------------------|
|                       | Dev. Exp. (%)                 | GCV           | p                | Dev. Exp. (%)                 | GCV           | p                |
| 0.5 degrees           | 67.5                          | 83.019        | <0.001           | 53.9                          | 46.927        | 0.75             |
| 1.0 degrees           | 67.7                          | 82.492        | <0.001           | 53.9                          | 46.899        | 0.21             |
| 2.5 degrees           | 68.4                          | 80.655        | <0.001           | 54.1                          | 46.741        | <0.01            |
| 5.0 degrees           | 68.7                          | 79.895        | <0.001           | 54.2                          | 46.608        | <0.001           |
| 10 degrees            | <b>69.0</b>                   | <b>79.214</b> | <b>&lt;0.001</b> | 54.1                          | 46.859        | 0.08             |
| 25 degrees            | 67.5                          | 82.795        | <0.001           | <b>54.9</b>                   | <b>45.988</b> | <b>&lt;0.001</b> |
| Best + HMS smoke flag | <b>69.1</b>                   | <b>79.025</b> | <b>&lt;0.001</b> | <b>55.1</b>                   | <b>45.959</b> | <b>&lt;0.001</b> |

Table 5. Quality of fit for GAMs using different FINN fire count predictors to predict background MDA8 O<sub>3</sub>.

|                       | Houston Bkgrd MDA8 O <sub>3</sub> |               |                  | El Paso Bkgrd MDA8 O <sub>3</sub> |               |                  |
|-----------------------|-----------------------------------|---------------|------------------|-----------------------------------|---------------|------------------|
|                       | Dev. Exp. (%)                     | GCV           | p                | Dev. Exp. (%)                     | GCV           | p                |
| 0.5 degrees           | 63.5                              | 60.402        | 0.05             | 51.0                              | 40.737        | 0.76             |
| 1.0 degrees           | 63.7                              | 60.14         | 0.001            | 51.0                              | 40.739        | 0.69             |
| 2.5 degrees           | 64.1                              | 59.389        | <0.001           | 51.2                              | 40.619        | 0.01             |
| 5.0 degrees           | <b>64.4</b>                       | <b>58.959</b> | <b>&lt;0.001</b> | 51.2                              | 40.621        | 0.04             |
| 10 degrees            | 64.4                              | 59.072        | <0.001           | 51.3                              | 40.619        | 0.01             |
| 25 degrees            | 64.0                              | 59.671        | <0.001           | <b>52.3</b>                       | <b>39.788</b> | <b>&lt;0.001</b> |
| Best + HMS smoke flag | <b>64.6</b>                       | <b>58.890</b> | <b>&lt;0.001</b> | <b>52.6</b>                       | <b>39.641</b> | <b>&lt;0.001</b> |

As in Section 4.1.1, we use the GAMs to calculate the MDA8 O<sub>3</sub> first using the actual HMS smoke flag and FINN fire counts, and then estimate a smoke-free case by setting the smoke flag to 0 for all days and setting the FINN fire count variables to their minimums on smoky days (30 for the ±10-degree Houston box and 400 for the ±25-degree El Paso box). The distribution of these differences on days where the HMS indicated smoke overhead are shown in Table 6. In general, these more advanced GAMs indicate a larger influence of smoke on background MDA8 O<sub>3</sub> in these urban areas that the smoke flag only GAMs did, averaging 6.1 ppbv in El Paso and 7.8 ppbv in Houston. In addition, while the El Paso differences between the background and maximum impacts of smoke follow the previous pattern of a decrease as the smoke enters the city (-1.6 ppbv on average), in Houston we now see a significant increase related to the fire predictors (+6.0 ppbv). These differences in smoke impact between the background and maximum MDA8 O<sub>3</sub> are statistically significant at  $p < 0.001$  (t-test and Kolmogorov-Smirnov test). It is unclear why these urban areas have such significant differences in the estimated smoke impact on urban chemistry. The decrease in El Paso could be due to NO titration of the O<sub>3</sub> from the fires, while the Houston results would suggest a significant impact of the fire-related VOCs on the urban chemistry.

Table 6. Change in MDA8 O<sub>3</sub> due to the presence of smoke as indicated by the HMS smoke flag in the GAMs trained on the meteorological predictors, the HMS smoke flag, and FINN fire counts.

|                             | <b>Houston MDA8 O<sub>3</sub></b> |            | <b>El Paso MDA8 O<sub>3</sub></b> |            |
|-----------------------------|-----------------------------------|------------|-----------------------------------|------------|
|                             | Bkgrd (ppbv)                      | Max (ppbv) | Bkgrd (ppbv)                      | Max (ppbv) |
| Minimum                     | 1.3                               | 2.4        | 2.7                               | 1.9        |
| 25 <sup>th</sup> Percentile | 5.8                               | 11.3       | 5.3                               | 3.3        |
| Median                      | 7.9                               | 13.6       | 6.1                               | 4.3        |
| Mean                        | 7.8                               | 13.8       | 6.1                               | 4.5        |
| 75 <sup>th</sup> percentile | 9.6                               | 16.9       | 6.9                               | 5.7        |
| Max                         | 18.4                              | 28.2       | 9.4                               | 8.8        |
| Std. Dev.                   | 3.0                               | 4.3        | 1.4                               | 1.4        |

#### 4.1.3 Geographic FINN fire count and emissions fits

To further investigate the influence of fire emissions on urban MDA8 O<sub>3</sub> in Houston and El Paso, we calculated total fire counts and emissions of multiple species in geographic regions near Texas: the Yucatan (YUC), all of Mexico (MEX), California (CA), and states bordering Texas (LA, AR, OK, NM). We then replaced the FINN fire count predictors used in Section 4.1.2 above with these new predictors one by one to find the FINN variable in each region that gave the best fit with MDA8 background and maximum O<sub>3</sub>. The best variables for each region and predictand are given in Table 7.

Table 7. Best FINN fire variable by geographic region.

| Region | Houston                         |  | El Paso                         |                                |
|--------|---------------------------------|--|---------------------------------|--------------------------------|
|        | Maximum MDA8 O <sub>3</sub>     | Background MDA8 O <sub>3</sub>           | Maximum MDA8 O <sub>3</sub>     | Background MDA8 O <sub>3</sub> |
| MEX    | Biomass burned (BMASS)          | Non-methane hydrocarbon (NMHC) emissions | BMASS                           | Xylene emissions               |
| YUC    | Fire Area                       | Fire Count                               | Fire Area                       | Fire Area                      |
| OK     | Fire Count                      | BMASS                                    | Fire Count                      | Fire Count                     |
| NM     | Fire Count                      | Fire Count                               | Fire Count                      | Fire Count                     |
| LA     | Fire Count                      | Fire Count                               | Hydroxyacetone (HYAC) emissions | CH <sub>3</sub> CN emissions   |
| AR     | Fire Count                      | NMHC emissions                           | Fire Count                      | Fire Count                     |
| CA     | NO <sub>x</sub> emissions as NO | Glycolaldehyde (GLYALD) emissions        | NO <sub>x</sub> emissions as NO | Fire Area                      |

The general FINN fire count predictors used in Section 4.1.2 were replaced with these geographic variables and the GAMs were rerun. Variables that were not significant at least  $p < 0.10$  were removed and the fits rerun. The results were:

- Houston Max  $O_3$  – Only MEX, AR, and NM kept as significant predictors. Total deviance explained was 68.2% with a GCV of 81.6, which is a better fit than the large-scale FINN fire count fit from Section 4.1.2. Increases in Mexican biomass burned and Arkansas fire counts were associated with increased  $O_3$  but saturated at relatively low values, while NM fire counts slightly decreased  $O_3$  (Figure 3).

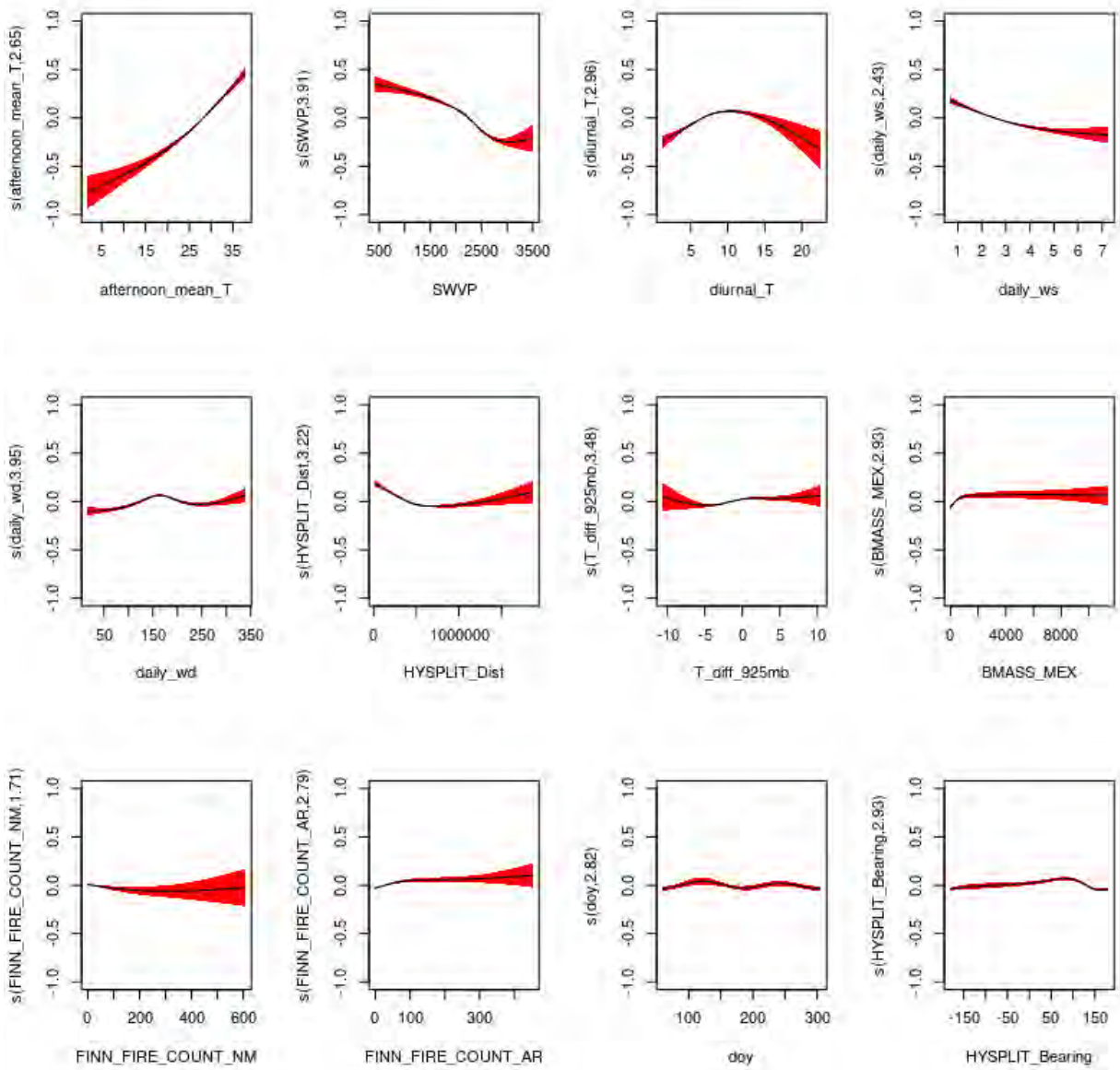


Figure 3. Smooth function fits for the log of maximum MDA8  $O_3$  in Houston.

- Houston Background O<sub>3</sub> – All variables were kept as significant predictors. Total deviance explained was 65.5% with a GCV of 57.9, which is a better fit than the large-scale FINN fire count fit from Section 4.1.2. All fire impacts were positive except for NM, with MEX and AR showing the largest impacts (Figure 4).

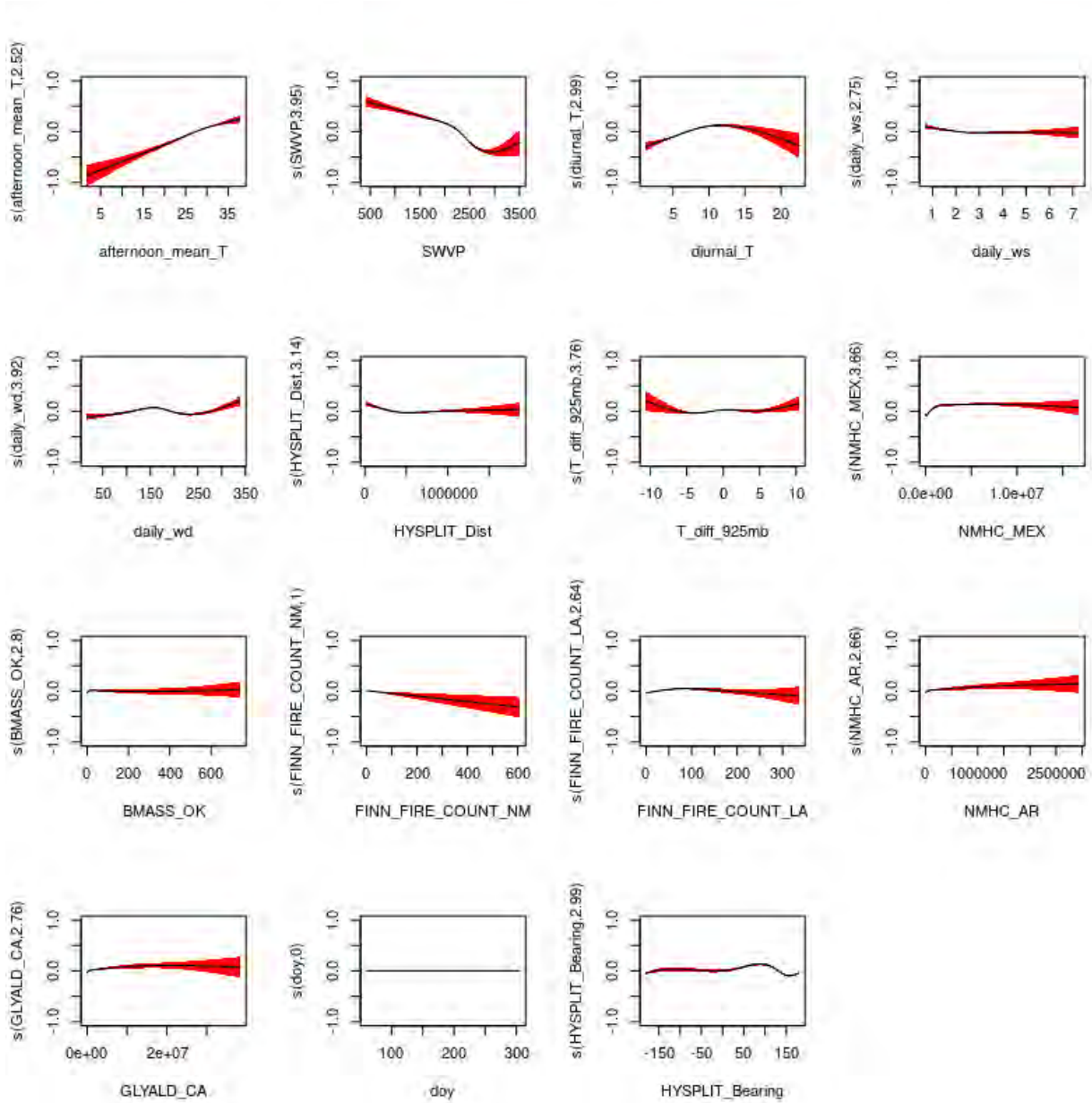


Figure 4. Smooth function fits for the log of background MDA8 O<sub>3</sub> in Houston.

- El Paso Max O<sub>3</sub> – AR was removed, but all other variables kept as significant predictors. Total deviance explained was 57.1% with a GCV of 44.43, which is a better fit than the large-scale FINN fire count fit from Section 4.1.2. Only the Mexico predictor had a large increase in O<sub>3</sub> and saturated quickly (Figure 5).

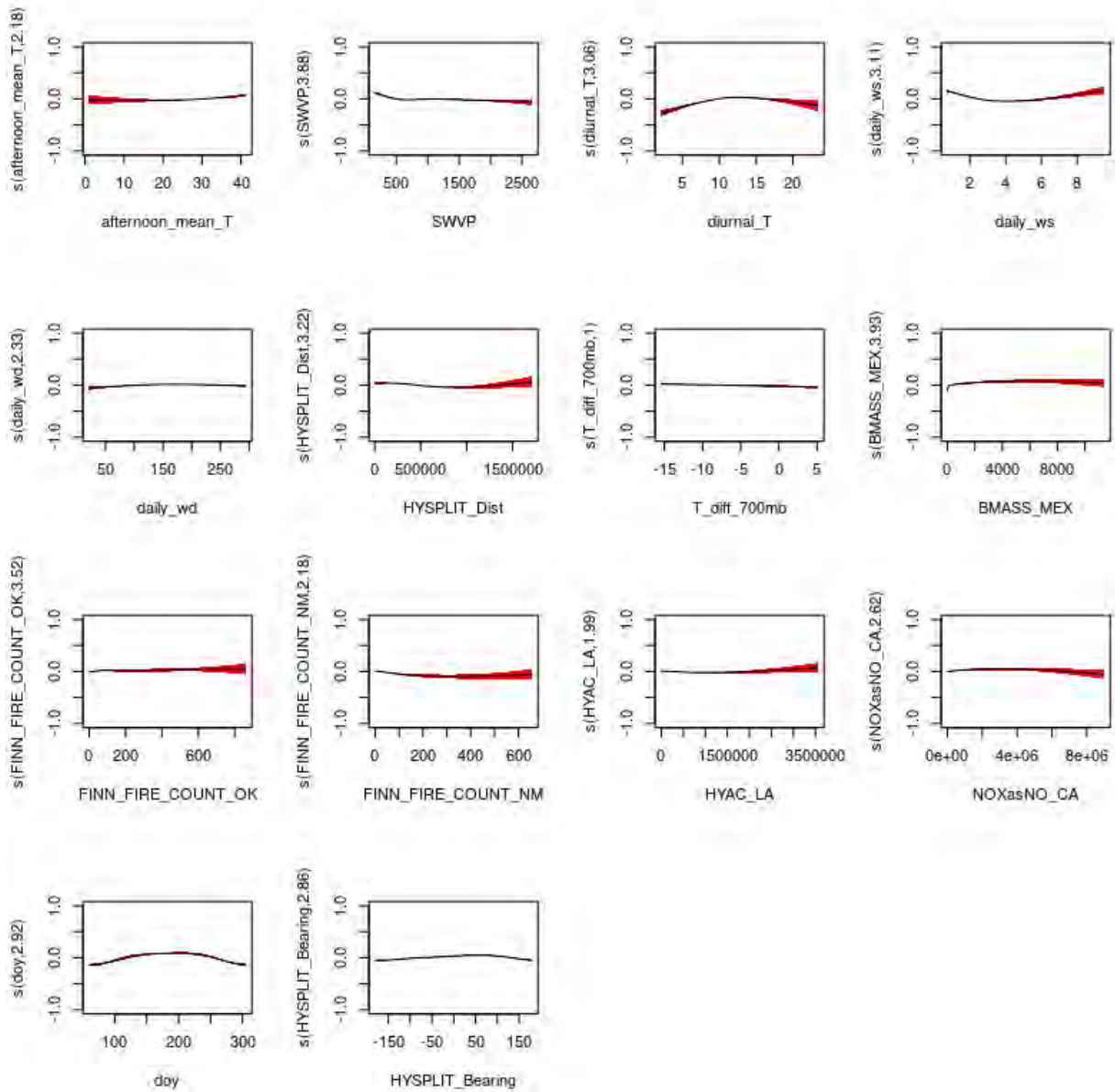


Figure 5. Smooth function fits for the log of maximum MDA8 O<sub>3</sub> in El Paso.

- El Paso Background O<sub>3</sub> – AR was removed, but all other variables kept as significant predictors. Total deviance explained was 54.4% with a GCV of 38.57, which is a better fit than the large-scale FINN fire count fit from Section 4.1.2. Mexico tended to increase O<sub>3</sub> while NM decreased it (Figure 6).

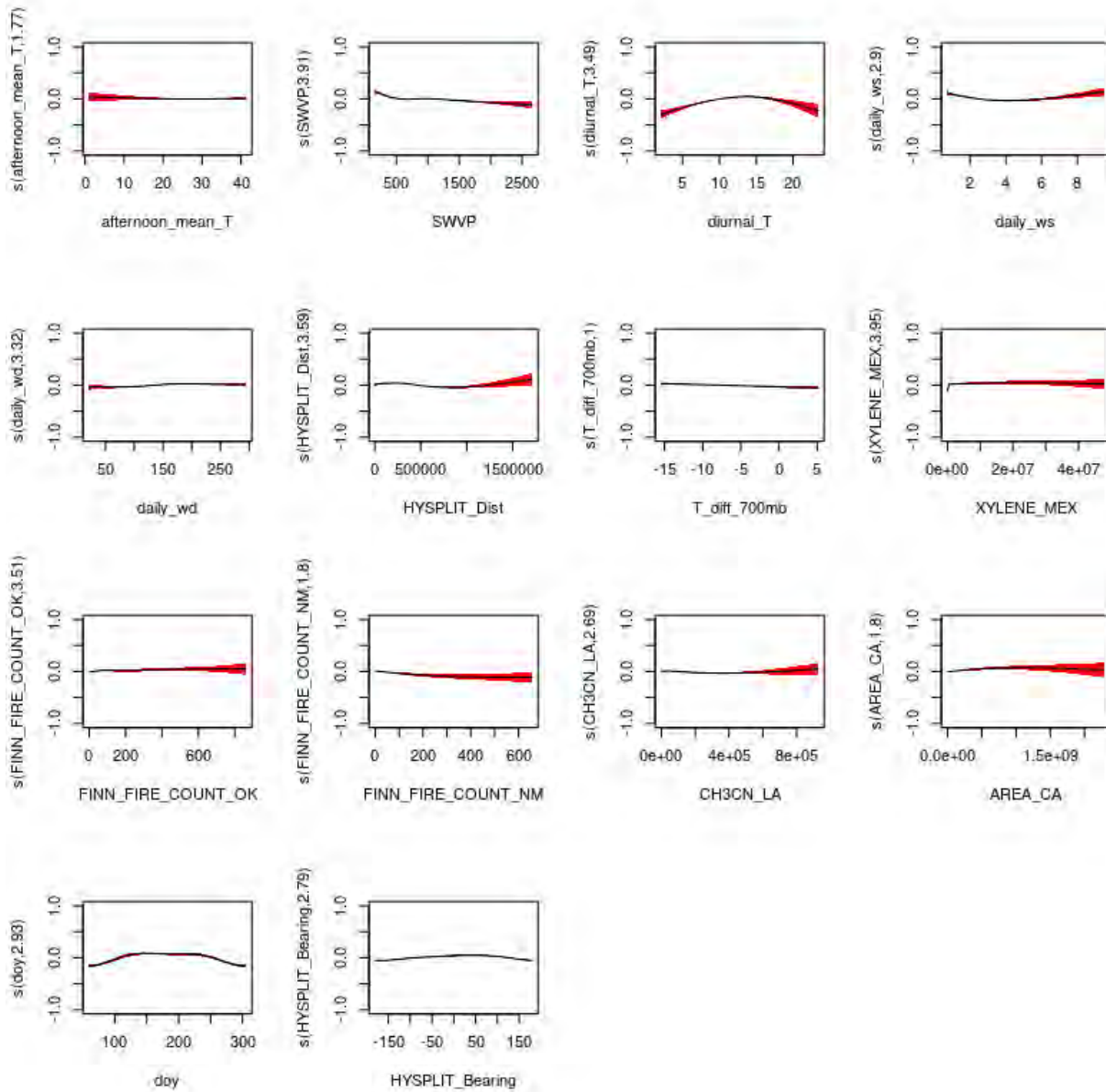


Figure 6. Smooth function fits for the log of background MDA8 O<sub>3</sub> in El Paso.

As before, we use the GAMs to calculate the MDA8 O<sub>3</sub> first using the actual HMS smoke flag and geographic FINN variables, and then estimate a smoke-free case by setting the smoke flag to 0 for all days and setting the geographic FINN variables to their minimums on smoky days. The distribution of these differences on days where the HMS indicated smoke overhead are shown in Table 8. In this case, the GAMs predict relatively large impacts of smoke on background and maximum MDA8 O<sub>3</sub> in both urban areas (means of 7-8 ppbv) with a slight decrease in the smoke related O<sub>3</sub> when the smoke enters the city (-0.9 ppbv mean for Houston, -0.2 ppbv mean for El Paso). The small changes as the



smoke enters the city are similar to the smoke flag only results from Section 4.1.1, but the absolute impact of smoke is estimated to be much higher in this fit.

Table 8. Change in MDA8 O<sub>3</sub> due to the presence of smoke as indicated by the HMS smoke flag in the GAMs trained on the meteorological predictors, the HMS smoke flag, and FINN geographic variables.

|                             | <b>Houston MDA8 O<sub>3</sub></b> |            | <b>El Paso MDA8 O<sub>3</sub></b> |            |
|-----------------------------|-----------------------------------|------------|-----------------------------------|------------|
|                             | Bkgrd (ppbv)                      | Max (ppbv) | Bkgrd (ppbv)                      | Max (ppbv) |
| Minimum                     | 1.0                               | 2.0        | 1.6                               | 0.3        |
| 25 <sup>th</sup> Percentile | 5.6                               | 5.3        | 5.5                               | 5.4        |
| Median                      | 7.7                               | 7.0        | 7.4                               | 7.2        |
| Mean                        | 8.0                               | 7.1        | 7.2                               | 7.0        |
| 75 <sup>th</sup> percentile | 9.8                               | 8.4        | 8.7                               | 8.5        |
| Max                         | 23.2                              | 20.5       | 13.0                              | 12.6       |
| Std. Dev.                   | 3.7                               | 2.8        | 2.1                               | 2.3        |

While the geographic FINN fits seem to have the best fitting statistics (deviance explained and GCV), the fact that they predict negative impacts for some areas suggests that they may be fitting significant amounts of noise. In addition, as the variables are not kept constant between the max and background fits, it is not clear if the deltas calculated for smoke entering the city are trustworthy.

#### 4.1.4 WRF-STILT footprint fits

The convolved WRF-STILT footprints with the FINN emissions at 0.01x0.01 degrees generally gave similar fits regardless of the specific species fit. Thus, here we focus on the results for FINN NO. The convolved footprints were highly significant predictors ( $p \ll 0.001$ ) of background and maximum MDA8 O<sub>3</sub> in Houston, but surprisingly were not significant predictors for El Paso. The deviance explained and GCV statistics for each fit were:

- Houston Maximum – Deviance explained 67.9%, GCV 81.9
- Houston Background – Deviance explained 64.2%, GCV 59.4
- El Paso Maximum – Deviance explained 54.2%, GCV 46.1
- El Paso Background – Deviance explained 51.8%, GCV 39.8

These fit statistics are generally worse than those using the FINN fire count variables directly in Sections 4.1.2 and 4.1.3, suggesting that the WRF-STILT footprints may not correctly represent the transport of biomass burning emissions to these urban areas.

As before, we use the GAMs to calculate the MDA8 O<sub>3</sub> first using the actual HMS smoke flag and NO footprints, and then estimate a smoke-free case by setting the smoke flag to 0 for all days and setting the NO footprints to their minimums on smoky days. The distribution of these differences on days where the HMS indicated smoke overhead are shown in Table 9. As only the Houston results had the footprints as significant predictors,

we focus on those. In this case, the GAMs predicted a mean impact of smoke on Houston background O<sub>3</sub> of 4.5 ppbv, increasing by 2.2 ppbv as the smoke entered the city.

Table 9. Change in MDA8 O<sub>3</sub> due to the presence of smoke as indicated by the HMS smoke flag in the GAMs trained on the meteorological predictors, the HMS smoke flag, and the WRF-STILT/FINN NO footprints.

|                             | <b>Houston MDA8 O<sub>3</sub></b> |            | <b>El Paso MDA8 O<sub>3</sub></b> |            |
|-----------------------------|-----------------------------------|------------|-----------------------------------|------------|
|                             | Bkgrd (ppbv)                      | Max (ppbv) | Bkgrd (ppbv)                      | Max (ppbv) |
| Minimum                     | -2.9                              | 1.2        | 1.6                               | 1.2        |
| 25 <sup>th</sup> Percentile | 3.4                               | 5.4        | 2.3                               | 1.7        |
| Median                      | 4.7                               | 6.6        | 2.6                               | 1.9        |
| Mean                        | 4.5                               | 6.7        | 2.7                               | 2.0        |
| 75 <sup>th</sup> percentile | 5.8                               | 8.3        | 3.1                               | 2.1        |
| Max                         | 10.22                             | 13.3       | 4.7                               | 5.8        |
| Std. Dev.                   | 1.9                               | 2.4        | 0.6                               | 0.6        |

Table 10 summarizes the mean results for Objective 1. Unfortunately, the results depend strongly on which set of fire predictors is used. For Houston, the range of impacts of fires on mean background MDA8 O<sub>3</sub> is 2.4 to 8.0 ppbv, with the change in O<sub>3</sub> impact as the smoke enters the city varying from -0.9 ppbv to +6.0 ppbv, with three out of four methods predicting an increase in mean O<sub>3</sub> as the smoke enters the city. In El Paso, the range of impacts of fires on mean background MDA8 O<sub>3</sub> is 2.4 to 7.2 ppbv, similar to Houston, with the change in mean O<sub>3</sub> impact as the smoke enters the city varying from -1.6 ppbv to -0.5 ppbv. The geographic fire variables from Sec. 4.1.3 give the best fitting statistics and predicts fire impacts of 7.0-8.0 ppbv in both urban areas, with a slight decrease in the impact when the smoke enters the city.

Table 10. Mean smoke impacts on background and maximum MDA8 O<sub>3</sub> in each urban area for different sets of smoke predictors.

|  | <b>Houston MDA8 O<sub>3</sub></b> |            | <b>El Paso MDA8 O<sub>3</sub></b> |            |
|--|-----------------------------------|------------|-----------------------------------|------------|
|  | Bkgrd (ppbv)                      | Max (ppbv) | Bkgrd (ppbv)                      | Max (ppbv) |
| Smoke flag only (Sec. 4.1.1)             | 2.4                               | 2.6        | 2.4                               | 1.9        |
| + large-scale fire counts (Sec. 4.1.2)   | 7.8                               | 13.8       | 6.1                               | 4.5        |
| + geographic fire variables (Sec. 4.1.3) | 8.0                               | 7.1        | 7.2                               | 7.0        |
| + WRF-STILT footprints (Sec. 4.1.4)      | 4.5                               | 6.7        | 2.7                               | 2.0        |

## 4.2 Objective 2: Ability of CAMx to simulate fire impacts

We used the updated dataset with the CAMx data (Section 2.4) to retrain the GAMs for maximum and background MDA8 O<sub>3</sub> for El Paso and Houston (total of four cases). The

significance of the “Is\_Model” factor variable was used to determine if the differences between the CAMx and ambient results were statistically significant. The model smooth functions and factor values were then examined for differences between the GAM trained with CAMx data and the ones without CAMx data, and the predicted impacts of smoke by each model were examined for differences.

### 4.2.1 El Paso Maximum MDA8 O<sub>3</sub>

Our early work (Section 4.1.2) had shown that combining the HMS smoke flag and the 25 degree FINN fire counts gave the best results for the ambient data for El Paso Maximum MDA8 O<sub>3</sub> values, and so those parameters were reused here. The “Is\_Model” variable was highly significant for this case (p<0.001), suggesting that the CAMx and ambient model results are significantly different. However, an examination of the smooth functions for each fit (Figure 7) shows very little difference between the smooth function fits for the cases with and without CAMx data, including for the dependence of maximum O<sub>3</sub> on the FINN fire counts. The parametric coefficient for HMS smoke flag also showed only small differences between the two GAMs (0.024 for ambient data only, 0.021 when CAMx data is added). These results tend to suggest that the difference between the CAMx predictions and the ambient data could be mostly explained by a constant fractional bias which is mostly accounted for by the Is\_Model factor variable coefficient.

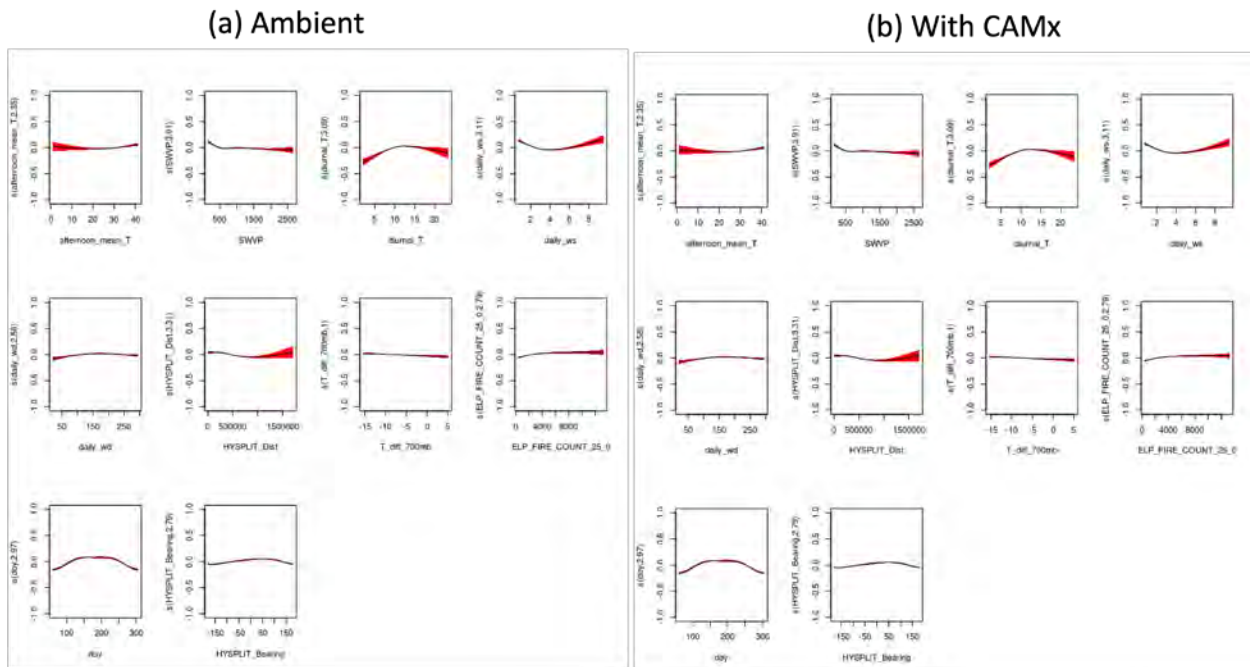


Figure 7. Smooth function fits for El Paso maximum MDA8 O<sub>3</sub> using (a) only ambient data and (b) using CAMx data with an Is\_Model factor variable.

We further examined the differences by (a) comparing the maximum MDA8 O<sub>3</sub> predictions for 2019 for different values of the Is\_Model variable to examine the fractional bias between the model and ambient data and (b) comparing the GAM predictions with and without the smoke variables for 2019 to examine how the predicted smoke impacts differ in the ambient data and the CAMx simulations. Table 11 shows the

differences in the GAM predictions of the ambient and CAMx data for 2019. The mean percentage difference is -8% (i.e., CAMx underestimated the true mean by 8%), but the differences are larger for high O<sub>3</sub> days (-10%) than for low O<sub>3</sub> days (-3%), suggesting CAMx significantly underestimates the peak O<sub>3</sub> events in El Paso, leading to the significance of the Is\_Model variable in the GAM fits.

Table 11. Ambient and CAMx GAM predictions for the 2019 maximum MDA8 O<sub>3</sub> (ppbv) for El Paso based on the GAM model with the Is\_Model variable.

|                             | Ambient<br>(Is_Model = 0) | CAMx<br>(Is_Model = 1) | % Difference |
|-----------------------------|---------------------------|------------------------|--------------|
| Minimum                     | 35.3                      | 34.1                   | -3%          |
| 25 <sup>th</sup> Percentile | 47.7                      | 44.5                   | -7%          |
| Median                      | 53.4                      | 49.7                   | -7%          |
| Mean                        | 52.7                      | 48.7                   | -8%          |
| 75 <sup>th</sup> percentile | 57.8                      | 53.1                   | -8%          |
| Max                         | 68.4                      | 61.8                   | -10%         |
| Std. Dev.                   | 6.9                       | 5.9                    |              |

Table 12 shows the difference in smoke impacts calculated for 2019 days where the HMS indicated smoke over El Paso. Note that this subset only includes 8 days. The GAMs trained on ambient data and the CAMx data make similar predictions for the fire impacts on these days, with the CAMx predictions generally being 0.3-0.4 ppbv smaller but showing no dependence with the strength of the ambient fire impact. This suggests that the CAMx predictions of MDA8 O<sub>3</sub> on fire days only slightly underpredict the actual impacts of fires on maximum MDA8 O<sub>3</sub> in El Paso.

Table 12. Estimated impact of smoke on the 2019 maximum MDA8 O<sub>3</sub> (ppbv) for El Paso when calculated from Ambient and CAMx data.

|                             | Ambient | CAMx |
|-----------------------------|---------|------|
| Minimum                     | 2.8     | 2.5  |
| 25 <sup>th</sup> Percentile | 4.0     | 3.7  |
| Median                      | 4.2     | 3.9  |
| Mean                        | 4.3     | 4.0  |
| 75 <sup>th</sup> percentile | 4.7     | 4.4  |
| Max                         | 5.6     | 5.2  |
| Std. Dev.                   | 0.8     | 0.8  |

#### 4.2.2 El Paso Background MDA8 O<sub>3</sub>

The “Is\_Model” variable was highly significant for El Paso background O<sub>3</sub> ( $p < 0.001$ ), suggesting that the CAMx and ambient model results are significantly different. However, an examination of the smooth functions for each fit (Figure 8) shows very little difference between the smooth function fits for the cases with and without CAMx data, including for the dependence of maximum O<sub>3</sub> on the FINN fire counts. The parametric coefficient for HMS smoke flag also showed only small differences between the two GAMs (0.036 for ambient data only, 0.031 when CAMx data is added). These results tend to suggest that

the difference between the CAMx predictions and the ambient data could be mostly explained by a fractional bias which is mostly accounted for by the Is\_Model factor variable coefficient.

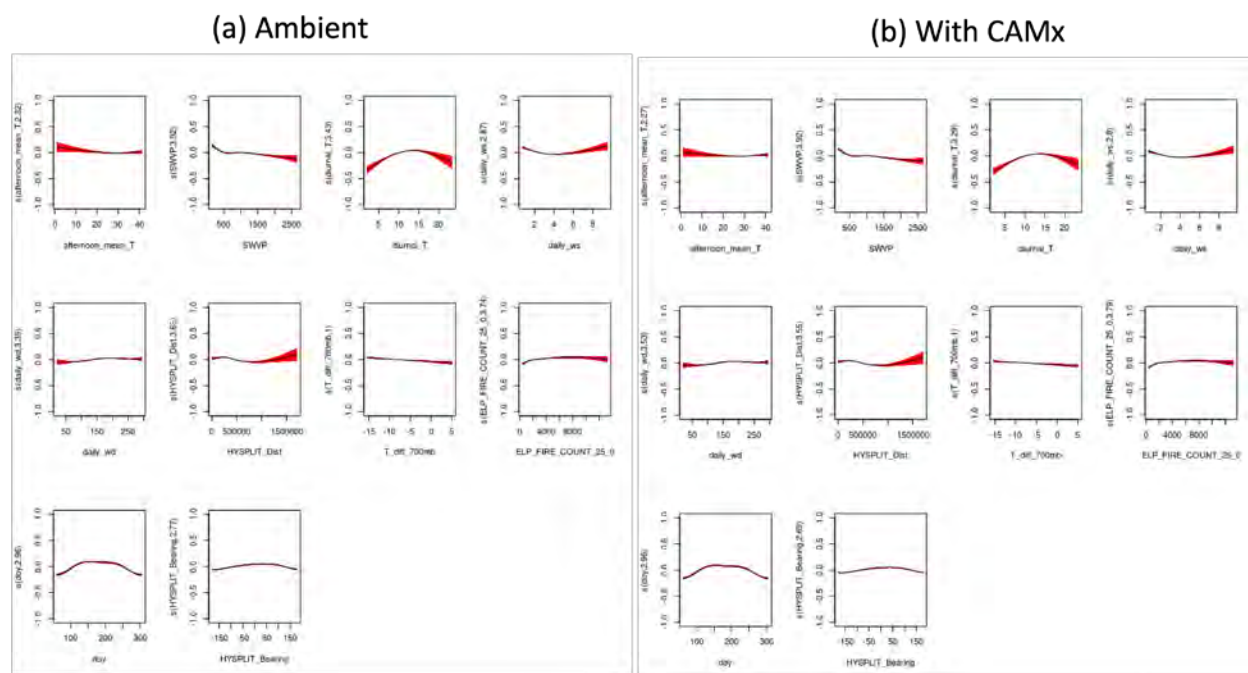


Figure 8. Smooth function fits for El Paso background MDA8 O<sub>3</sub> using (a) only ambient data and (b) using CAMx data with an Is\_Model factor variable.

We further examined the differences by (a) comparing the maximum MDA8 O<sub>3</sub> predictions for 2019 for different values of the Is\_Model variable to examine the fractional bias between the model and ambient data and (b) comparing the GAM predictions with and without the smoke variables for 2019 to examine how the predicted smoke impacts differ in the ambient data and the CAMx simulations. Table 13 shows the differences in the GAM predictions of the ambient and CAMx data for 2019. The mean percentage difference is -4% (i.e., CAMx underestimated the true mean by 4%), but the differences are generally larger for high O<sub>3</sub> days (-5%) than for low O<sub>3</sub> days (-1%).

Table 13. Ambient and CAMx GAM predictions for the 2019 background MDA8 O<sub>3</sub> (ppbv) for El Paso based on the GAM model with the Is\_Model variable.

|                             | Ambient<br>(Is_Model = 0) | CAMx<br>(Is_Model = 1) | % Difference |
|-----------------------------|---------------------------|------------------------|--------------|
| Minimum                     | 33.7                      | 32.1                   | -5%          |
| 25 <sup>th</sup> Percentile | 42.3                      | 42.0                   | -1%          |
| Median                      | 48.2                      | 46.2                   | -4%          |
| Mean                        | 47.6                      | 45.9                   | -4%          |
| 75 <sup>th</sup> percentile | 52.5                      | 50.6                   | -4%          |
| Max                         | 61.4                      | 58.1                   | -5%          |
| Std. Dev.                   | 6.3                       | 5.9                    |              |

Table 14 shows the difference in smoke impacts calculated for 2019 days where the HMS indicated smoke over El Paso. Note that this subset only includes 8 days. The GAMs trained on ambient data and the CAMx data make similar predictions for the fire impacts on these days, with the CAMx predictions generally being 0.2-0.4 ppbv smaller but showing no dependence with the strength of the ambient fire impact. This suggests that the CAMx predictions of MDA8 O<sub>3</sub> on fire days only slightly underpredict the actual impacts of fires on background MDA8 O<sub>3</sub> in El Paso.

Table 14. Estimated impact of smoke on the 2019 background MDA8 O<sub>3</sub> (ppbv) for El Paso when calculated from Ambient and CAMx data.

|                             | Ambient | CAMx |
|-----------------------------|---------|------|
| Minimum                     | 4.6     | 4.4  |
| 25 <sup>th</sup> Percentile | 6.3     | 6.0  |
| Median                      | 6.5     | 6.1  |
| Mean                        | 6.4     | 6.0  |
| 75 <sup>th</sup> percentile | 6.6     | 6.3  |
| Max                         | 7.6     | 7.2  |
| Std. Dev.                   | 0.8     | 0.8  |

#### 4.2.3 Houston Maximum MDA8 O<sub>3</sub>

Our previous work (Deliverable 2, Task 1) had shown that combining the HMS smoke flag and the 10 degree FINN fire counts gave the best results for the ambient data for Houston Maximum MDA8 O<sub>3</sub> values, and so those parameters were reused here. The “Is\_Model” variable was **not** significant for this case ( $p > 0.1$ ), suggesting that the CAMx and ambient model results are substantially the same. An examination of the smooth functions for each fit (Figure 9) shows very little difference between the smooth function fits for the cases with and without CAMx data, including for the dependence of maximum O<sub>3</sub> on the FINN fire counts. The parametric coefficient for HMS smoke flag also showed only small differences between the two GAMs (0.033 for ambient data only, 0.034 when CAMx data is added).

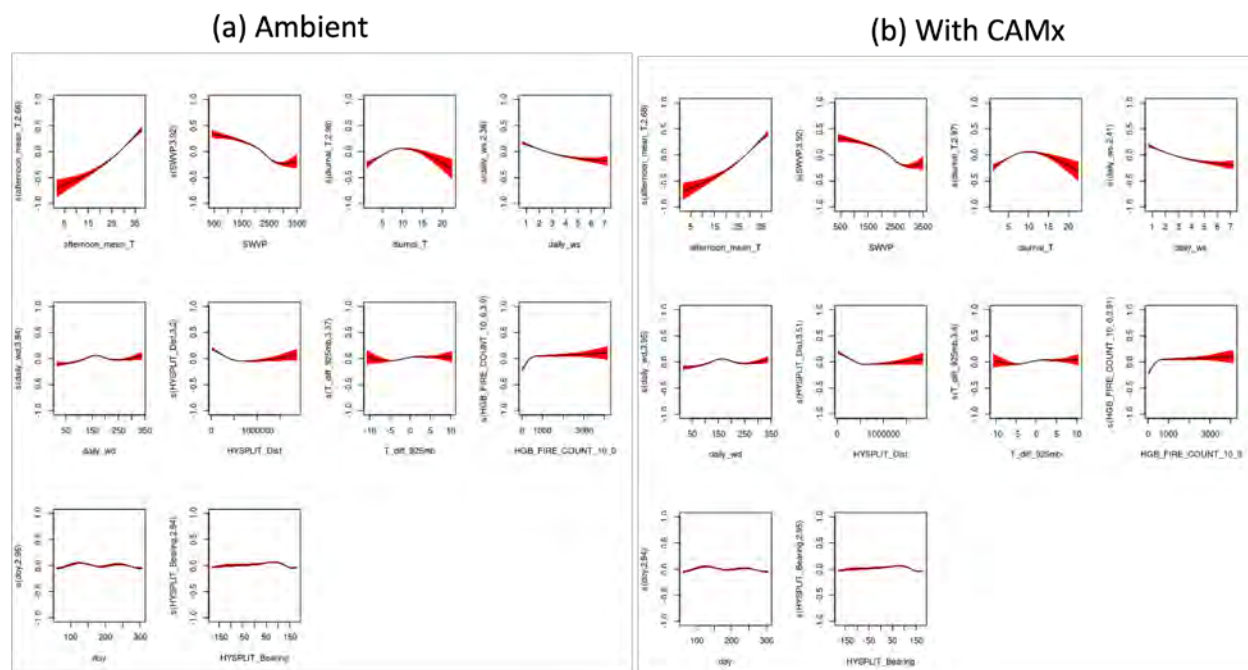


Figure 9. Smooth function fits for Houston maximum MDA8 O<sub>3</sub> using (a) only ambient data and (b) using CAMx data with an Is\_Model factor variable.

We further examined the differences by (a) comparing the maximum MDA8 O<sub>3</sub> predictions for 2019 for different values of the Is\_Model variable to examine the fractional bias between the model and ambient data and (b) comparing the GAM predictions with and without the smoke variables for 2019 to examine how the predicted smoke impacts differ in the ambient data and the CAMx simulations. Table 15 shows the differences in the GAM predictions of the ambient and CAMx data for 2019. The mean percentage difference is 3% (i.e., CAMx overestimated the true mean by 3%), but the differences are fairly constant with large changes in ambient O<sub>3</sub>, consistent with the lack of significance for the Is\_Model factor.

Table 15. Ambient and CAMx GAM predictions for the 2019 maximum MDA8 O<sub>3</sub> (ppbv) for Houston based on the GAM model with the Is\_Model variable.

|                             | Ambient<br>(Is_Model = 0) | CAMx<br>(Is_Model = 1) | % Difference |
|-----------------------------|---------------------------|------------------------|--------------|
| Minimum                     | 27.7                      | 28.2                   | 2%           |
| 25 <sup>th</sup> Percentile | 42.7                      | 43.7                   | 2%           |
| Median                      | 50.2                      | 51.2                   | 2%           |
| Mean                        | 52.4                      | 53.9                   | 3%           |
| 75 <sup>th</sup> percentile | 61.3                      | 62.5                   | 2%           |
| Max                         | 82.9                      | 84.1                   | 1%           |
| Std. Dev.                   | 12.5                      | 12.6                   |              |

Table 16 shows the difference in smoke impacts calculated for 2019 days where the HMS indicated smoke over Houston. Note that this subset only includes 35 days. The GAMs trained on ambient data and the CAMx data make similar predictions for the fire impacts on these days, with the CAMx predictions generally being 0.2-0.4 ppbv larger but showing no dependence with the strength of the ambient fire impact. This suggests that the CAMx predictions of MDA8 O<sub>3</sub> on fire days only slightly underpredict the actual impacts of fires on maximum MDA8 O<sub>3</sub> in Houston.

Table 16. Estimated impact of smoke on the 2019 maximum MDA8 O<sub>3</sub> (ppbv) for Houston when calculated from Ambient and CAMx data.

|                             | Ambient | CAMx |
|-----------------------------|---------|------|
| Minimum                     | 9.4     | 11.0 |
| 25 <sup>th</sup> Percentile | 12.7    | 12.9 |
| Median                      | 15.3    | 15.6 |
| Mean                        | 15.6    | 15.8 |
| 75 <sup>th</sup> percentile | 18.3    | 18.1 |
| Max                         | 21.5    | 21.8 |
| Std. Dev.                   | 3.4     | 3.3  |

#### 4.2.4 Houston Background MDA8 O<sub>3</sub>

The “Is\_Model” variable was highly significant for Houston background O<sub>3</sub> ( $p < 0.001$ ), suggesting that the CAMx and ambient model results are significantly different. However, an examination of the smooth functions for each fit (Figure 10) shows very little difference between the smooth function fits for the cases with and without CAMx data, including for the dependence of maximum O<sub>3</sub> on the FINN fire counts. However, the parametric coefficient for HMS smoke flag is different between the two GAMs (0.058 for ambient data only, 0.063 when CAMx data is added).



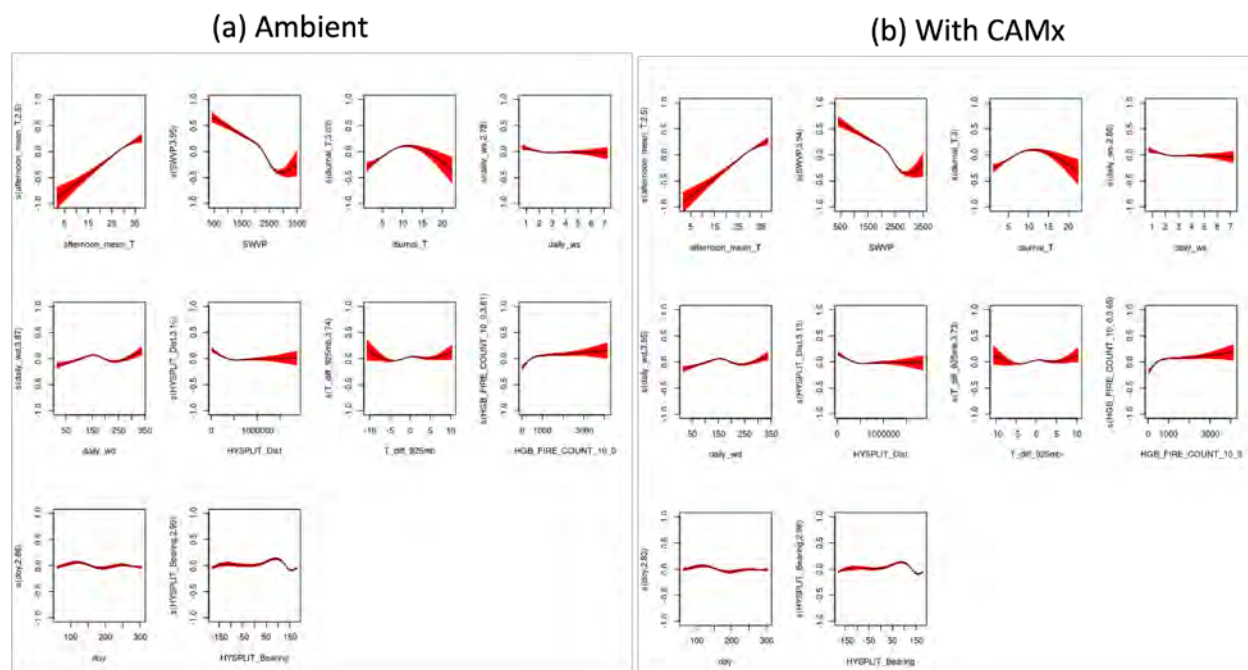


Figure 10. Smooth function fits for Houston background MDA8 O<sub>3</sub> using (a) only ambient data and (b) using CAMx data with an Is\_Model factor variable.

We further examined the differences by (a) comparing the maximum MDA8 O<sub>3</sub> predictions for 2019 for different values of the Is\_Model variable to examine the fractional bias between the model and ambient data and (b) comparing the GAM predictions with and without the smoke variables for 2019 to examine how the predicted smoke impacts differ in the ambient data and the CAMx simulations. Table 17 shows the differences in the GAM predictions of the ambient and CAMx data for 2019. The mean percentage difference is 21% (i.e., CAMx overestimated the true mean by 21%), with little dependence on the value of the ambient background O<sub>3</sub>. This large overestimate of background O<sub>3</sub> by CAMx is very different than the results for El Paso background O<sub>3</sub>.

Table 17. Ambient and CAMx GAM predictions for the 2019 background MDA8 O<sub>3</sub> (ppbv) for Houston based on the GAM model with the Is\_Model variable.

|                             | Ambient<br>(Is_Model = 0) | CAMx<br>(Is_Model = 1) | % Difference |
|-----------------------------|---------------------------|------------------------|--------------|
| Minimum                     | 16.4                      | 20.2                   | 23%          |
| 25 <sup>th</sup> Percentile | 23.9                      | 28.9                   | 21%          |
| Median                      | 28.9                      | 35.5                   | 23%          |
| Mean                        | 31.0                      | 37.6                   | 21%          |
| 75 <sup>th</sup> percentile | 37.2                      | 45.4                   | 22%          |
| Max                         | 57.6                      | 67.0                   | 16%          |
| Std. Dev.                   | 9.1                       | 11.0                   |              |

Table 18 shows the difference in smoke impacts calculated for 2019 days where the HMS indicated smoke over Houston. Note that this subset only includes 39 days. The GAMs trained on ambient data and the CAMx data make similar predictions for the fire impacts on these days, with the CAMx predictions generally being 2 ppbv larger but showing no dependence with the strength of the ambient fire impact. This suggests that the CAMx predictions of MDA8 O<sub>3</sub> on fire days overestimate the actual impacts of fires on background MDA8 O<sub>3</sub> in Houston.

Table 18. Estimated impact of smoke on the 2019 background MDA8 O<sub>3</sub> (ppbv) for Houston when calculated from Ambient and CAMx data.

|                             | Ambient | CAMx |
|-----------------------------|---------|------|
| Minimum                     | 5.6     | 8.4  |
| 25 <sup>th</sup> Percentile | 8.1     | 10.1 |
| Median                      | 9.2     | 11.1 |
| Mean                        | 9.7     | 11.6 |
| 75 <sup>th</sup> percentile | 10.9    | 13.0 |
| Max                         | 16.1    | 18.1 |
| Std. Dev.                   | 2.4     | 2.3  |

## 5 Quality Assurance

The processing and analysis scripts used in this project were inspected by a team member not involved in their creation for accuracy. All automated calculations and at least 10% of manual calculations will be inspected for correctness. This meets the requirement of Level III QAPPs that 10% of the data must be inspected.

Expert judgement was used to evaluate the reasonableness of the GAM fits for O<sub>3</sub> and STILT footprints. No concerning results were noted in these reviews.

The GAM fits for PM<sub>2.5</sub> show significant quality issues. The residuals are not normally distributed and show evidence of heteroskedacity. Various variable transforms did not remove these issues. Thus, the results of the PM<sub>2.5</sub> GAM analysis should be treated with caution, and only used to generate hypotheses about the smoke and dust impacts on PM<sub>2.5</sub> in Texas that need to be confirmed via other methods.

As the quality of the information, including secondary data, was not evaluated by EPA, the below disclaimer applies to all project deliverables:

*Disclaimer: The information contained in this report or deliverable has not been evaluated by EPA for this specific application.*

## 6 Conclusions

We performed a statistical analysis using generalized additive models (GAMs) to see how fires impacted background and maximum concentrations of  $O_3$  and  $PM_{2.5}$  in Houston and El Paso. Our results suggest that on days when the HMS indicated smoke over Houston and El Paso, the daily average  $PM_{2.5}$  was elevated by 1.4-2.6  $\mu\text{g}/\text{m}^3$  on average (background and maximum) while the background MDA8  $O_3$  was elevated by 2.4-8 ppbv on average. Unfortunately, the results depend strongly on which set of fire predictors is used. For Houston, the change in  $O_3$  impact as the smoke enters the city varies from -0.9 ppbv to +6.0 ppbv, with three out of four methods predicting an increase in mean  $O_3$  as the smoke enters the city. In El Paso, the change in mean  $O_3$  impact as the smoke enters the city varies from -1.6 ppbv to -0.5 ppbv. The geographic fire variables from Sec. 4.1.3 give the best fitting statistics and predicts fire impacts of 7.0-8.0 ppbv in both urban areas, with a slight decrease in the impact when the smoke enters the city.

We also performed a statistical analysis using generalized additive models (GAMs) to see if the CAMx predictions were consistent with the impact of fires on background and maximum concentrations of  $O_3$  in Houston and El Paso. For El Paso, our analysis suggested that there were statistically significant differences between CAMx and the ambient data, but further analysis showed that the predicted impacts of fires in both cases were very similar. For Houston, however, the differences between CAMx and the ambient data fits were not statistically significant for maximum  $O_3$ , but the CAMx data strongly overestimates the background  $O_3$  for Houston on both smoky and non-smoky days.

Since CAMx generally appears to give similar predictions for the impacts of smoke as the ambient data, there is little need to identify areas for improvement as called for in Objective 3 of this project. The exception is for the impacts of smoke on Houston background  $O_3$ , where CAMx predicts a 2 ppb larger impact. This is likely related to the general large overestimate of background  $O_3$  by CAMx in Houston but may also be due to errors in the chemistry as emissions from the Yucatan interact with halogens over the Gulf.

In addition, our results showed that CAMx overestimates Houston background  $O_3$  on both smoky and non-smoky days, suggesting that further work needs to be done on ozone-destroying halogen emissions and chemistry and on the biogenic emissions upwind of Houston. Similarly, the underpredictions of maximum  $O_3$  in El Paso suggest that further work is needed on CAMx emissions for El Paso and Ciudad Juarez and the  $O_3$  chemistry within the combined urban area.

## 7 Recommendations for Further Study

Future work should focus on finding ways to better determine the best set of smoke predictors for use in statistical studies such as this, with a focus on high tail events where smoke could lead to an exceedance of air quality standards using methods from Brown-Steiner et al. (2021). While the predictions of smoke impact on  $O_3$  from CAMx appear to be reasonable based on this study, our results suggest that further work is needed to (a)

address the overestimate of Houston background  $O_3$  on both smoky and non-smoky days and (b) the underpredictions of maximum  $O_3$  in El Paso.

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