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

AQRP Project 22-003

Presented to: University of Texas-Austin and Texas Commission on Environmental Quality

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## Three Chemical Stages of Smoke Ozone (O<sub>3</sub>) Formation



Near-Source Chemistry (0-6 hr)

Long-range Transport (6-48 hr)

Rapid  $O_3$  formation Depletion of initial NO<sub>x</sub> and HRVOCs Net O<sub>3</sub> formation settles to ~ 0.2 dO<sub>3</sub>/dCO

**Mixing with Urban Air** 

## Mixing of smoke organics with fresh $NO_x$ from the fires can increase urban $O_3$ formation

Alvarado et al., Smoke Chemistry, in Peterson, D. L., McCaffrey, S. M., & Patel-Weynand, T. (2022). Wildland Fire Smoke in the United States: A Scientific Assessment (p. 341). Springer Nature.

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# Estimates of the increase in $O_3$ when smoke mixes with urban emissions (Brey and Fischer, ES&T) 2016



Change in O<sub>3</sub> mixing ratio

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## **Our Previous Work on Smoke Influences on O<sub>3</sub> in Houston**



Impacts of	of 8-20 ppb	$0 V O_3!$			LAUNCH TRAILER	CO (ppbv)	O₃ (ppbv)	NO (ppb)	)	NO <sub>2</sub> (ppb)	v) NOy (ppb)	/)
					Mean (HMS Smoke)	295.5 (n=3151)	30.39 (n=4016)	4.421 (n=	3947)	16.14 (n=3468)	17.38 (n=3979)	
	JONES FOREST	CO (ppbv)	O3 (ppbv)		Mean (HMS No smoke)	207.0 (n=1141)	21.57 (n=1823)	2.373 (n=	1759)	9.607 (n=1575)	9.743 (n=1832)	
	Mean (HMS Smoke)	197.8 (n=2782)	38.1 (n=4016)		Diff (95%CI)/Signif?	88.49 (81.51, 95.48)/Y	8.811 (7.88 9.735)/Y	36, 2.049 (1.6 2.402)/Y	i95 <i>,</i>	6.537(5.8 7.184)/Y	90, 7.643 (7.0 8.257)/Y	28,
	Mean (HMS No smoke)	135.4 (n=839)	26.3 (n=1837)	- T	antsville	$\langle \langle \rangle \rangle$				, , , , , , , , , , , , , , , , , , ,		
Diff (95%Cl)/Signif? 62.4 11.8 (59.1,65.8)/Y (10.7,12.3)/Y					1							
			The Woodlards Beaumont	int	SMITH POINT	03	(ppbv)	NO (ppbv)	NO <sub>2</sub> (ppbv)			
					O ton		Mean (HMS Smoke)	42. (n=	2 3071)	0.400 (n=2660)	3.21 (n=2647)	
				Rosenber	g, Land	and the second s		Mean (HMS No smoke)	21. (n=	3 1084)	0.566 (n=1088)	2.12 (n=1084)
			Jon Jon		Galve Lake Jackson	ston		Diff (95%Cl)/Signif?	20. 21.	9 (20.3 <i>,</i> 6)/Y	-0.167 (-0.372, 0.0400)/N	1.09 (0.844, 1.33)/Y
				Bay City	det							
		co (mala)	(marked)		A NO Inch					1		

MOODY TOWER	CO (ppbv)	O <sub>3</sub> (ppbv)	NO (ppbv)	NO <sub>2</sub> (ppbv)	NOy (ppbv)	SO <sub>2</sub> (ppbv)
Mean (HMS Smoke)	219.9 (n=3153)	34.35 (n=4045)	3.138 (n=4003)	11.19 (n=4004)	15.97 (n=4003)	0.7899 (n=3360)
Mean (HMS No smoke)	154.3 (n=1651)	21.95 (n=1984)	1.364 (n=1994)	5.724 (n=1995)	8.100 (n=1995)	0.2883 (n=1631)
Diff (95%CI)/Signif?	65.60 (60.54, 70.66)/Y	12.40 (11.52, 13.28)/Y	1.774 (1.498, 2.051)/Y	5.470(5.091, 5.849)/Y	7.872(7.315, 8.429)/Y	0.5017(0.4354, 0.5680)/Y

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## **Our Previous Statistical Studies of O<sub>3</sub> Formation in Texas**







Pernak et al., AAQR, 2019. https://doi.org/10.4209/aaqr.2018.12.0464



Brown-Steiner et al., AAQR, 2021. https://doi.org/10.4209/aaqr.210077

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- 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 two Texas urban areas (Houston and El Paso).
- 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.



## **Ambient Air Quality Data**

- Surface air quality data from TAMIS
- Calculated maximum daily 8-hour average (MDA8)  $O_3$  mixing ratios and daily average  $PM_{2.5}$  concentrations for each site
  - Sites separated into background (for sites on the outskirts of the city) and urban (for sites near the city core).
  - Background: the minimum value of MDA8  $O_3$  and daily average  $PM_{2.5}$  from background sites
  - Maximum: Maximum concentrations in each region (including background sites).

## **Meteorological Predictors**

- Afternoon mean temperature (°C, afternoon\_mean\_T, 1-4 PM CST)
- 2. Diurnal temperature change (°C, diurnal\_T)
- 3. Daily average wind speed (m/s, daily\_ws)
- Daily average wind direction (degrees clockwise from North, daily\_wd)
- 5. Daily average water vapor density (g/m<sup>3</sup>, SWVP)
- 6. Morning surface temperature difference (1200 UTC) (temperature at 925 or 700 mb-temperature at surface at 1200 UTC) (°C, T\_dif\_925mb or T\_dif\_700mb)

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- 7. Transport direction (degrees clockwise from North, HYSPLIT\_Bearing)
- 8. Transport distance (m, HYSPLIT\_dist)

Variables 1-5 were calculated from the surface meteorological data in the Texas Air Monitoring Information System (TAMIS).

Variable 6 was calculated from the the Integrated Global Radiosonde Archive (IGRA Version 2).

Variables 7 and 8 were calculated from 24-hour HYSPLIT back-trajectories (300 m AGL, start at local solar noon) driven with 12 km NAM data.







The smoke flag files were generated from NOAA Hazard Mapping System (HMS) smoke polygons for 2012 – 2021 that were converted to the GOES CONUS grid for colocation with the urban area.

# Fire and Smoke Predictors: FINN Fire Counts and Emissions



## • Large-scale

- Used Fire Inventory from NCAR (FINN v2.5, Wiedinmyer et al., 2011, McDonald-Buller et al., 2015, 1 km resolution)
- Determined 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).

## Geographic

 Sum fire counts, area, biomass burned, and species emissions for Mexico (MEX), Yucatan (YUCATAN), states bordering Texas (NM, AR, OK, LA) and California (CA)

## Scholarity of observed concentrations to emissions upwind (i.e

Accumulated "footprint" estimating impact of fire emissions on  $PM_{2.5}$  concentrations at Manaus.

 $10^{-3}$ 

55°W

ppmv/(micromole m-2 s-1))

50°W

10<sup>-2</sup>

45°W

 $10^{-1}$ 

40°W

 $10^{0}$ 

5°N

0°

5°S

10°S

75°W

10<sup>-6</sup>

70°W

10<sup>-5</sup>

65°W

10-4

60°W

from all other fires.

Convolved 3-day WRF-STILT footprints with  $0.1 \times 0.1$  degree FINN v2.5 fire emissions for NO, NO<sub>2</sub>, CO, and CO<sub>2</sub> to get estimates of fire emissions impact.

Results were very similar regardless of species, so focused on NO.

Fire and Smoke Predictors: WRF-STILT Footprints

WRF-STILT traces 500 stochastic particle back-trajectories to determine the sensitivity of observed concentrations to emissions upwind (i.e., the footprint, left).



2010. Green is from fires in Amazonas, red







- 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.



 GAMs are extensions of multiple linear regression models that fit unknown non-linear functions of predictors

$$g(\mu_i) = \beta_o + f_1(x_{i,1}) + f_2(x_{i,2}) + \cdots + f_n(x_{i,n}) + f_p(D_i) + W_d$$

- 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 and fire predictors (except HMS smoke flag) 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  $O_3$  and  $PM_{2.5}$  concentrations as these are usually log-normally distributed.

## **Checking Quality of Fit**



### Good Fit, El Paso O<sub>3</sub>



Histogram of residuals







### Poor Fit, Houston PM<sub>2.5</sub>



Histogram of residuals

Response vs. Fitted Values







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

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## **Smoke Flag Tests: MDA8 O<sub>3</sub> Impacts**



	Houston M	IDA8 O <sub>3</sub>	El Paso MDA8 O <sub>3</sub>		
	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.	0.6	0.6	0.2	0.2	

- O<sub>3</sub> is increased by 1.2-4.8 ppbv when HMS says there is smoke over the city
- Less than impact of smoke inferred when not controlling for meteorology.
- Small increase in impact when smoke enters Houston, small decrease in El Paso

## Smoke Flag Tests: Daily Average PM<sub>2.5</sub> Impacts



- Houston PM<sub>2.5</sub> Background: 1.9-2.6 μg/m<sup>3</sup>
- Houston PM<sub>2.5</sub> Max: 1.5-2.3 μg/m<sup>3</sup>
- El Paso  $PM_{2.5}$  Background: 1.7-2.5 µg/m<sup>3</sup>
- El Paso PM<sub>2.5</sub> Max: 1.5-2.6 μg/m<sup>3</sup>

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## FINN Large-Scale Fire Count Tests: Max O<sub>3</sub> Fits



	Houst	on Max M	IDA8 O <sub>3</sub>	El Pa	so Max MD	A8 O <sub>3</sub>
	Dev.	GCV	р	Dev.	GCV	р
	Exp.			Exp.		
	(%)			(%)		
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	69.0	79.214	<0.001	54.1	46.859	0.08
25 degrees	67.5	82.795	<0.001	54.9	45.988	<0.001
Best + HMS smoke flag	69.1	79.025	<0.001	55.1	45.959	<0.001



ELP\_FIRE\_COUNT\_25\_0

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## FINN Large-Scale Fire Count Tests: Bkgrd O<sub>3</sub> Fits



	Housto	n Bkgrd N	IDA8 O <sub>3</sub>	El Pas	so Bkgrd M	DA8 0 <sub>3</sub>
	Dev.	GCV	р	Dev.	GCV	р
	Exp.			Exp.		
	(%)			(%)		
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	64.4	58.959	<0.001	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	52.3	39.788	<0.001
Best + HMS	64.6	58.890	<0.001	52.6	39.641	<0.001
smoke flag						



## FINN Large-Scale Fire Count Tests: MDA8 O<sub>3</sub> Impacts



	Houston	MDA8 O <sub>3</sub>	El Paso MDA8 O <sub>3</sub>		
	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	

- Adding FINN fire counts greatly increases the estimated impact of smoke on O<sub>3</sub>, more in line with uncorrected BC2 estimates from previous work
- Large increase in impact when smoke enters Houston, small decrease in El Paso

## **FINN Geographic Predictor Tests: Best variables**



	Hou	iston	El Paso		
	Maximum MDA8	Background	Maximum MDA8	Background	
Region	0 <sub>3</sub>	MDA8 O <sub>3</sub>	0 <sub>3</sub>	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	Glycoladehyde (GLYALD) emissions	NO <sub>x</sub> emissions as NO	Fire Area	

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





# 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 largescale FINN fire counts.

Increases in Mexican biomass burned and Arkansas fire counts were associated with increased O3 but saturated at relatively low values, while NM fire counts slightly decreased  $O_3$ 

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## 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.

All fire impacts were positive except for NM, with MEX and AR showing the largest impacts (Figure 4).

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## El Paso Maximum 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.

Only the Mexico predictor had a large increase in O<sub>3</sub> and saturated quickly.

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1.0

-50 50 150

HYSPLIT Bearing

-150

1.0

100

200

doy

300

## 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.

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0.0

1.0

-150 -50 50

HYSPLIT Bearing

150

s(HYSPLIT

0.0

0

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200

doy

300



	Houston I	MDA8 O <sub>3</sub>	El Paso MDA8 O <sub>3</sub>		
	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	

- Gives best fit with data of tested predictors
- Significant smoke impacts (mean 7-8 ppbv)
- Small decrease in impact when smoke enters Houston, small decrease in El Paso



- The convolved footprints were highly significant predictors (p << 0.001) 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, suggesting that the WRF-STILT footprints may not correctly represent the transport of biomass burning emissions to these urban areas.



	Houston I	MDA8 O <sub>3</sub>	El Paso MDA8 O <sub>3</sub>		
	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	

- Lower impacts than FINN fits, but poorer fit
- Shape of response similar to Mexican FINN variables
- Significant smoke impacts (mean 7-8 ppbv)
- Large increase in impact when smoke enters Houston, small decrease in El Paso



	Houstor	Houston MDA8 O <sub>3</sub>		MDA8 O <sub>3</sub>
	Bkgrd	Max (ppbv)	Bkgrd	Max
	(ppbv)		(ppbv)	(ppbv)
Smoke flag only	2.4	2.6	2.4	1.9
+ large-scale fire counts	7.8	13.8	6.1	4.5
+ geographic fire variables	8.0	7.1	7.2	7.0
+ WRF-STILT footprints	4.5	6.7	2.7	2.0

## Houston

- Mean background MDA8 O<sub>3</sub> is increased 2.4 to 8.0 ppbv by smoke
- Change in O<sub>3</sub> impact as the smoke enters the city -0.9 ppbv to +6.0 ppbv
- El Paso
  - Mean background MDA8 O<sub>3</sub> is increased 2.4 to 7.2 ppbv by smoke
  - Change in  $O_3$  impact as the smoke enters the city -1.6 ppbv to -0.5 ppbv.

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# Objective 2: Ability of CAMx to simulate fire impacts

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- Use the FINN large scale predictors and the smoke flag
  - Houston: FINN fire counts within 10 degrees
  - El Paso: FINN fire counts within 25 degrees
- Include Is\_Model variable in the fit as a factor
- If Is\_Model is statistically significant, the CAMx simulation is different from the ambient data
- Determine source of difference
  - Examine smooth fits and factor coefficients for differences
  - Look at difference in GAM predictions for 2019 for different O<sub>3</sub> levels
  - Look at differences in predicted smoke impacts

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





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## El Paso Maximum MDA8 O<sub>3</sub>: Total O<sub>3</sub> Predictions



	Ambient (ppbv) (Is_Model = 0)	CAMx (ppbv) (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	

 CAMx underestimates maximum O<sub>3</sub> in El Paso, with underestimates more severe at high O<sub>3</sub> levels

## El Paso Maximum MDA8 O<sub>3</sub>: Smoke O<sub>3</sub> Predictions



	Ambient (ppbv)	CAMx (ppbv)
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

- Estimated smoke impacts are very similar in ambient data and CAMx simulations (within 0.4 ppbv)
- This, plus similarity of the smooth function fits and the smoke\_flag coefficient, suggest CAMx does a reasonable job modeling the impact of smoke on maximum O<sub>3</sub> in El Paso, even while underestimating the absolute values

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



(a) Ambient (b) With CAMx 1.0 10 mean\_T,2.32) \_T,2.27) lal\_T,3.43) ws,2.87) 0.5 0.5 0.5 0.5 0.5 0.5 T,3.29) 0.5 0.5 s(SWVP,3.92) ws,2.8) s(SWVP.3.92) 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 s(daily\_ s(diu 0.5 0.5 -0.5 0.5 -0.5 0.5 0.5 0.5 s(af 1.0 0 0 0 š 0 0 0 0 0 10 20 30 40 500 1500 2500 5 10 15 20 2 4 6 8 30 1500 10 15 20 4 6 0 10 20 40 500 2500 5 2 8 afternoon\_mean\_T SWVP diurnal\_T daily\_ws SWVP afternoon\_mean\_T diurnal T daily\_ws FIRE\_COUNT\_25\_0,3.74) 10 10 COUNT\_25\_0,3.79 0 s(HYSPLIT\_Dist, 3.65) (HYSPLIT\_Dist, 3.55) 700mb,1) 0.5 0.5 0.5 0.5 0.5 1), 1) 0.5 s(daily\_wd,3.35) 0.5 0.5 s(daily\_wd,3.53) 200 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 통 ŧ -0.5 -0.5 -0.5 -0.5 Ë 끮 0.5 -0.5 0.5 0.5 Ĕ s(ELP\_ -1.0 (ELP 0 0 0 10 0 0 0 150 250 1500000 4000 8000 50 0 500000 -15 -10 -5 0 5 0 150 250 1500000 -15 -10 -5 0 4000 8000 50 0 500000 5 0 HYSPLIT Dist T\_diff\_700mb ELP FIRE COUNT 25 0 daily\_wd daily\_wd HYSPLIT\_Dist T\_diff\_700mb ELP\_FIRE\_COUNT\_25\_0 Is\_Model variable highly significant ng,2.77) (69) 0.5 0.5 ng.2.0 But fits are similar 0.5 0.5 s(doy,2.96) s(doy,2.96) 0.0 s(HYSPLIT\_Be 0.0 YSPLIT\_Bea 0.0 0.0 Smoke\_flag coefficients similar ۲ 0.5 0.5 0.5 0.5 (0.036 ambient, 0.031 CAMx) Ĩ 0 -1.0 0 0 100 200 300 -150 -50 50 150 100 200 300 -150 -50 50 150 doy HYSPLIT Bearing HYSPLIT\_Bearing doy

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## El Paso Background MDA8 O<sub>3</sub>: Total O<sub>3</sub> Predictions



	Ambient (ppbv) (Is_Model = 0)	CAMx (ppbv) (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	

 CAMx underestimates background O<sub>3</sub> in El Paso, but percentage underestimate is relatively constant

## El Paso Background MDA8 O<sub>3</sub>: Smoke O<sub>3</sub> Predictions

	Ambient (ppbv)	CAMx (ppbv)
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

- As with maximum, estimated smoke impacts are very similar in ambient data and CAMx simulations (within 0.4 ppbv), suggesting CAMx does a reasonable job
- Both suggest a  $\sim$  2 ppbv loss of O<sub>3</sub> when smoke enters El Paso

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



(a) Ambient (b) With CAMx 1.0 n\_T,2.66) 0.5 0.5 0.5 0.5 0.5 nal\_T,2.97) ws.2.36) 0.5 ws,2.41) 0.5 0.5 s(SWVP,3.92) 5) 0.0 0.0 0.0 0.0 0.0 WP,3 0.0 0.0 0.0 -0.5 0.5 0.5 s (diur 0.5 0.5 0.5 0.5 0.5 0 0 5 15 25 1500 2500 3500 5 10 15 20 1 2 3 4 5 6 7 35 500 15 25 35 500 1500 2500 3500 10 15 20 1 2 3 4 5 6 7 5 5 afternoon mean T SWVP diurnal T daily\_ws SWVP afternoon mean T diurnal T daily\_ws COUNT\_10\_0,3.9) 1.0 0.3.9 Dist, 3.2) st,3.51) 37 0.5 s(T\_diff\_925mb,3.4) 9 0.5 0.5 0.5 ily\_wd,3.94) 0.5 0.5 0.5 'n 95) wd,3 (HYSPLIT\_Di 0.0 0.0 0.0 0.0 s(HYSPLIT\_ 0.0 0.0 0.0 0.0 FIRE ŧ s(da -0.5 0.5 0.5 0.5 0.5 -0.5 -0.5 0.5 0 0 0 0 0 1000000 -10 -5 0 5 10 50 150 250 350 0 1000 3000 0 50 150 250 350 1000000 -10 -5 0 5 10 0 1000 3000 0 daily wd HYSPLIT Dist T diff 925mb HGB FIRE COUNT 10 0 daily\_wd HYSPLIT\_Dist T\_diff\_925mb HGB\_FIRE\_COUNT\_10\_0 10 ng,2.94) Is\_Model variable **NOT** significant ullet0.5 0.5 9,2 0.5 0.5 s(doy,2.95) s(doy,2.94) Fits are similar 0.0 0.0 s(HYSPLIT\_Be 0.0 0.0 0.5 -0.5 0.5 0.5 Smoke\_flag coefficients similar ullet0 0 (0.033 ambient, 0.034 CAMx) 100 200 300 -150 -50 50 150 200 300 -150 -50 50 150 100 HYSPLIT\_Bearing doy doy HYSPLIT\_Bearing

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## Houston Maximum MDA8 O<sub>3</sub>: Total O<sub>3</sub> Predictions



	Ambient (ppbv) (Is_Model = 0)	CAMx (ppbv) (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	

• CAMx has small (2%) overestimates in Houston, constant through distribution

## Houston Maximum MDA8 O<sub>3</sub>: Smoke O<sub>3</sub> Predictions

	Ambient (ppbv)	CAMx (ppbv)
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

• Estimated smoke impacts are very similar in ambient data and CAMx simulations (within 0.3 ppbv except for minimum), suggesting CAMx does a reasonable job

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





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## Houston Background MDA8 O<sub>3</sub>: Total O<sub>3</sub> Predictions



	Ambient (ppbv) (Is_Model = 0)	CAMx (ppbv) (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	

CAMx has large overestimates of background O<sub>3</sub> in Houston, causing the Is\_Model variable to be significant

## Houston Background MDA8 O<sub>3</sub>: Smoke O<sub>3</sub> Predictions



	Ambient (ppbv)	CAMx (ppbv)
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

- CAMx predicts 2 ppbv more background O<sub>3</sub> impact of smoke in Houston than in ambient data
- CAMx suggests a net O<sub>3</sub> increase of 4 ppbv when the smoke enters the city, ambient data suggests 6 ppbv





- Only Houston Maximum MDA8  $O_3$  shows no significant difference between ambient and CAMx data when evaluated with the GAMs
- Only Houston Background MDA8 O<sub>3</sub> shows significant (> 1 ppbv) different between smoke impacts
- Houston Background MDA8  $O_3$  is also strongly (> 20%) overestimated in CAMx
- El Paso Maximum MDA8  $O_3$  is underestimated by CAMx, with a more severe underestimate at high  $O_3$  levels (-10%).

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# Objective 3: Directions for CAMx Modeling Improvements

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- Smoke impacts on  $O_3$  were similar in ambient data and CAMx data except for Houston background  $O_3$ , which was overestimated (2 ppb) in CAMx.
  - Since this impact seems mainly due to transport from Mexico/Yucatan, this could be due to errors in initial fire emissions, the formation of  $O_3$  in the Yucatan plume, or the chemistry over the Gulf during transport.
  - May also be related to overestimate of Houston background  $O_3$  in CAMx

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# Conclusions and Future Work

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## Conclusions



- 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 µg/m<sup>3</sup> on average
  - The background MDA8 O3 was elevated by 2.4-8 ppbv on average.
- 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.
  - 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.
- For El Paso, our CAMx 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, 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 and overestimates the smoke impact on background O<sub>3</sub> by 2 ppbv.

## Limitations of this Study



- Difficult to separate impacts of meteorology from smoke
  - Leads to smoke impact predictions depending strongly on what smoke predictors are included
- Looked at all levels of HMS smoke equally, did not separate heavy, medium, and light
- Only had 2019 CAMx data available
  - Longer runs using EQUATES dataset could help in evaluation with statistical models
- Did not include ambient measurements of precursor species (NO<sub>x</sub>, VOCs), firerelated species (CO, HCN), or PM<sub>2.5</sub> speciation (OC, EC)
  - Reliance on HMS to identify smoke days may introduce error due to lack of vertical information
  - But these measurements are limited to a small number of sites and days





- 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<sub>3</sub> 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<sub>3</sub> on both smoky and non-smoky days and (b) the underpredictions of maximum O<sub>3</sub> in El Paso.

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