

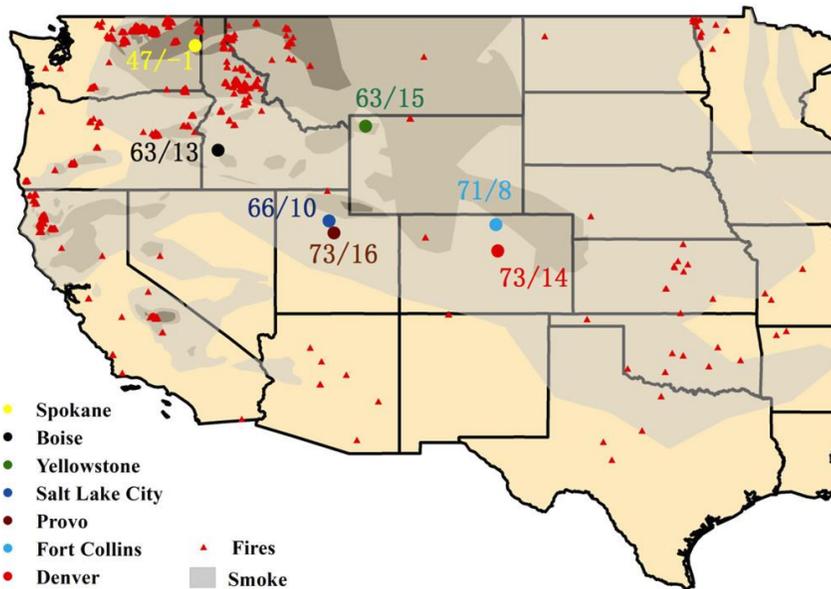
# Using 0-D photochemical modeling to understand smoke impacts on $O_3$

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# Introduction and Background

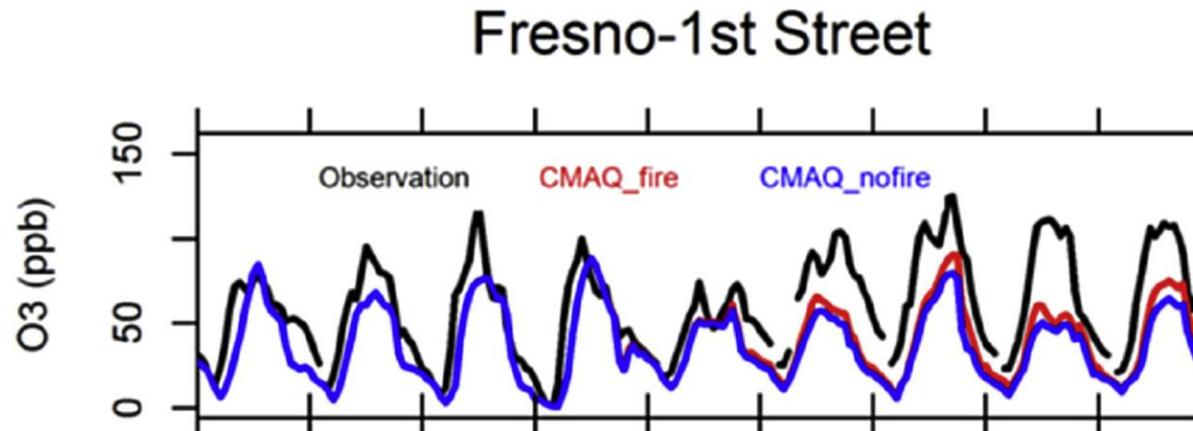
- Previous studies have used statistical modeling to quantify the additional amount of  $O_3$  produced due to wildfire smoke (e.g., Jaffe et al., 2004, 2013; Lu et al., 2016; Gong et al., 2017; McClure & Jaffe, 2018)
  - **Typical approach:** Generalized Additive Models (**GAMs**) – a form of machine learning
    - Estimates  $[O_3]$  due to smoke, but it tells us nothing about the  $O_3$  formation mechanism or the effect of smoke on concentrations of  $O_3$  precursors



- Figure from Gong et al. (2017)
- First value = observed maximum daily 8-hour average (**MDA8**)  $[O_3]$
- Second value = GAM-predicted  $[O_3]$  attributable to wildfire smoke

# Introduction and Background

- **Historically:** 3-D chemical transport models (**CTMs**) poorly simulate wildfire smoke impacts on atmospheric chemistry (e.g., Baker et al., 2016; Cai et al., 2016; Lu et al., 2016; Jaffe et al., 2018)



- Figure from Cai et al. (2016)
- Used the Community Multiscale Air Quality (**CMAQ**) model to investigate the effect of wildfire smoke on O<sub>3</sub> and other chemical species in California during June 2008

## Important points:

- Statistical models = only indicate **how much** O<sub>3</sub> is produced due to wildfire smoke
- CTMs = poorly simulate wildfire smoke impacts on the chemistry of O<sub>3</sub> and other pollutants

**For these reasons:** the chemical processes leading to O<sub>3</sub> enhancements in urban areas affected by wildfire smoke are **not** well-understood

- Important because many urban areas have difficulty meeting the O<sub>3</sub> National Ambient Air Quality Standard (**NAAQS**) of 70 parts per billion (**ppb**)

**To address this research gap:** the effect of wildfire smoke on O<sub>3</sub> production is being assessed for an urban site in Bakersfield, CA using field observations and a photochemical box model

- Photochemical box model = Framework for 0-D Atmospheric Modeling (**FOAM**)
- Bakersfield, CA = first case we chose to examine (will be looking at other cases for other cities)

## 4 main steps (additional details on subsequent slides):

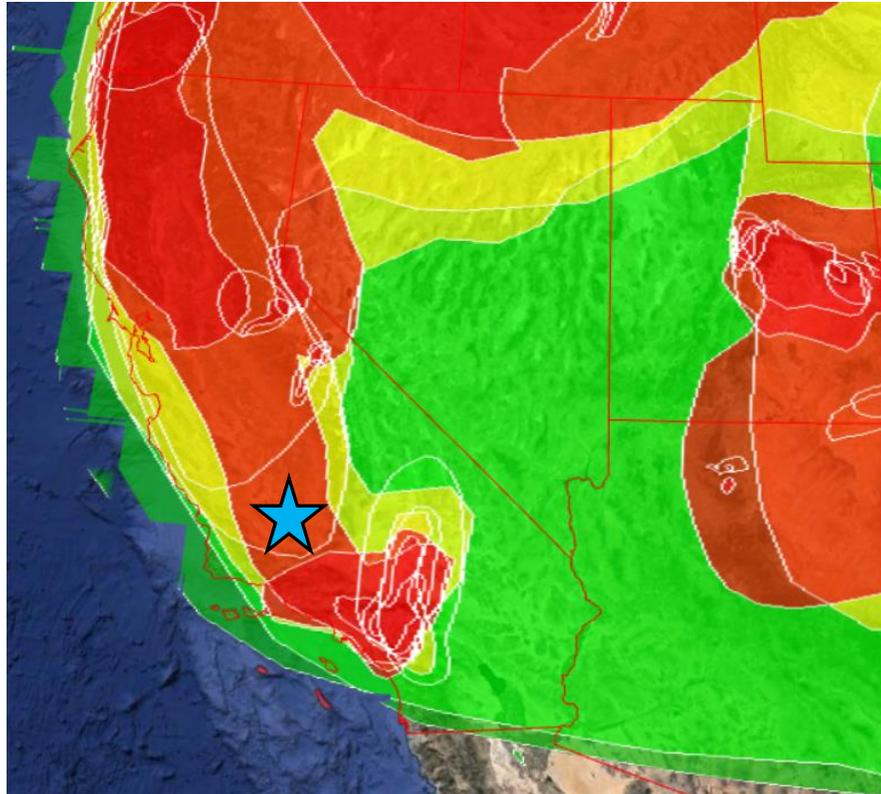
1. Identify a policy-relevant **smoke case** (MDA8 [O<sub>3</sub>] > 70 ppb) and a **non-smoke case**
  - Both cases needed to have similar meteorological conditions
2. Constrain F0AM with available observations
3. Specify background concentrations of selected pollutants for **smoke** and **non-smoke** days
4. Use the output from the F0AM simulations to assess smoke impacts on O<sub>3</sub>

# Methodology – case study selection details

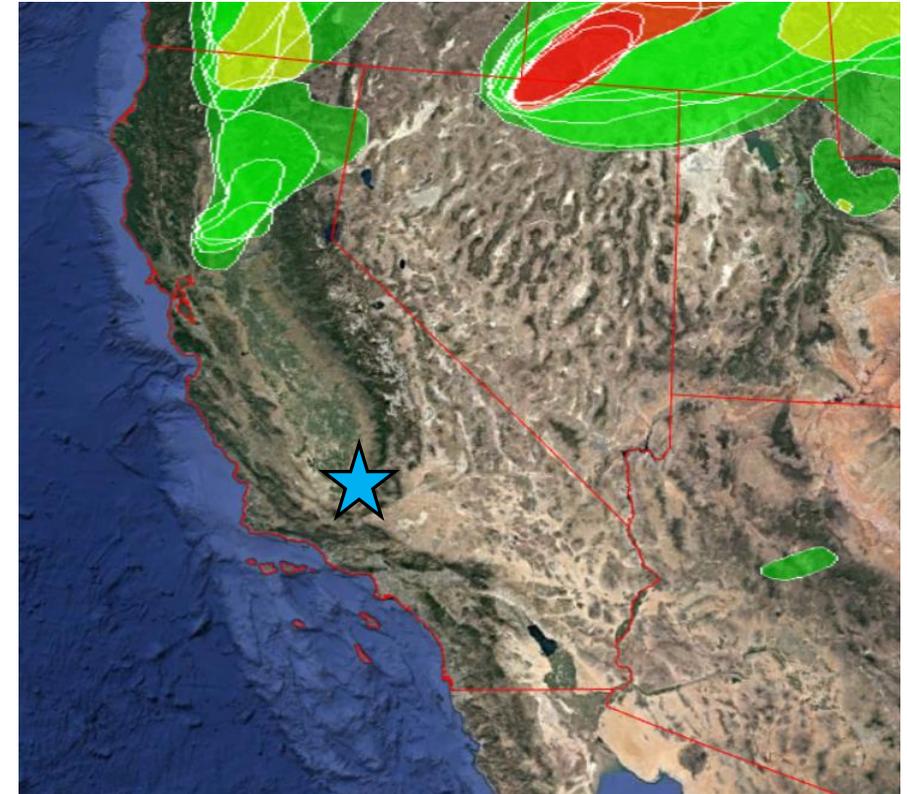
**Measurement site:** Bakersfield Municipal Airport (35.33° N, 119° W)

- The Hazard Mapping System Fire and Smoke Product (**HMS FSP**) was used to find the **smoke case (8/8/2018)** and the **non-smoke case (7/8/2018)**

Smoke case:



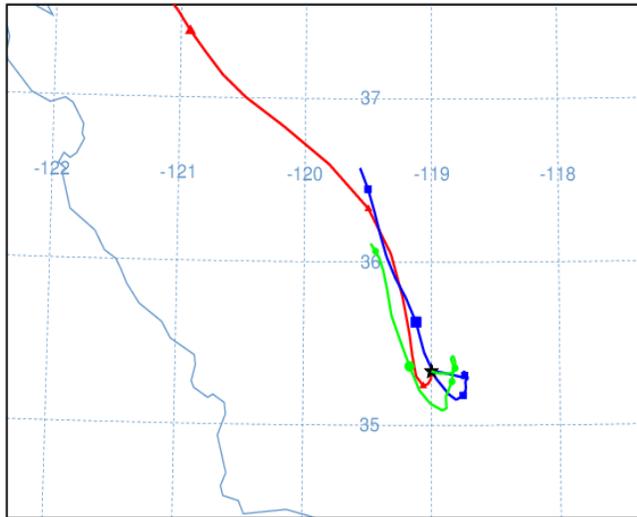
Non-smoke case:



# Comparison of **smoke** and **non-smoke** days

- The **smoke** and **non-smoke** days = characterized by similar meteorological conditions
- **Therefore:** differences in [O<sub>3</sub>] and other pollutants = likely due to **chemical** processes

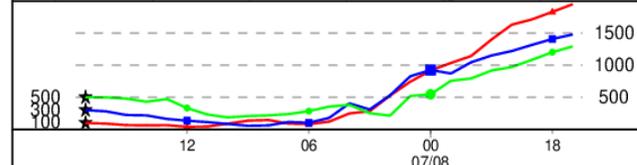
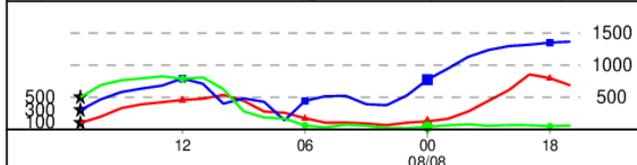
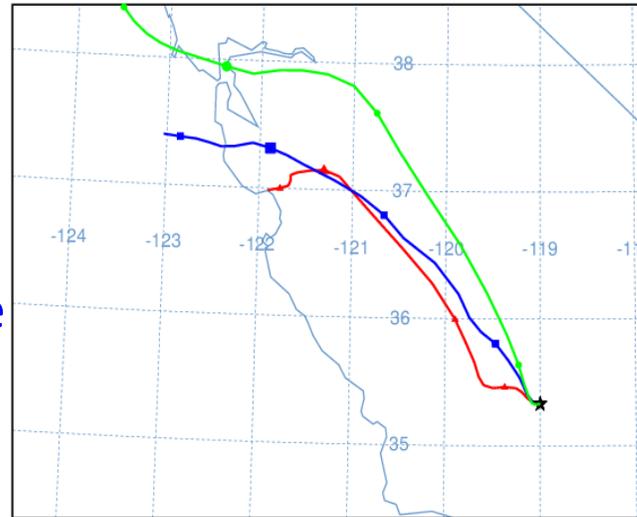
NOAA HYSPLIT MODEL  
Backward trajectories ending at 1700 UTC 08 Aug 18  
HRRR Meteorological Data



Smoke case:

Non-smoke case:

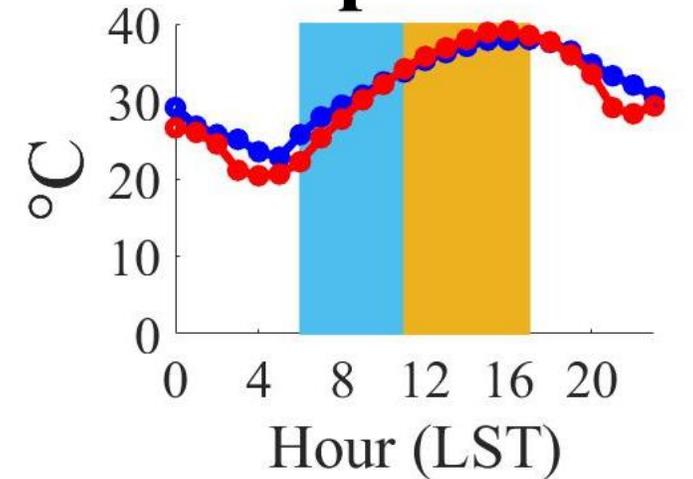
NOAA HYSPLIT MODEL  
Backward trajectories ending at 1700 UTC 08 Jul 18  
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Job ID: 143161 Job Start: Mon Sep 28 18:14:03 UTC 2020  
Source 1 lat.: 35.331612 lon.: -118.999961 hgts: 100, 300, 500 m AGL  
Trajectory Direction: Backward Duration: 24 hrs  
Vertical Motion Calculation Method: Model Vertical Velocity  
Meteorology: 1200Z 8 Aug 2018 - HRRR.V1

Job ID: 127117 Job Start: Tue Sep 29 23:08:06 UTC 2020  
Source 1 lat.: 35.331612 lon.: -118.999961 hgts: 100, 300, 500 m AGL  
Trajectory Direction: Backward Duration: 24 hrs  
Vertical Motion Calculation Method: Model Vertical Velocity  
Meteorology: 1200Z 8 Jul 2018 - HRRR.V1

## Temperature



Morning = 6:00-10:00 LST

Daytime = 11:00-17:00 LST

## Observations used to initialize FOAM:

- $O_3$ , carbon monoxide (**CO**), nitric oxide (**NO**), nitrogen dioxide (**NO<sub>2</sub>**), total volatile organic compound (**VOC**), and speciated concentrations of ~50 different VOCs
- Meteorological parameters – temperature, pressure, and relative humidity

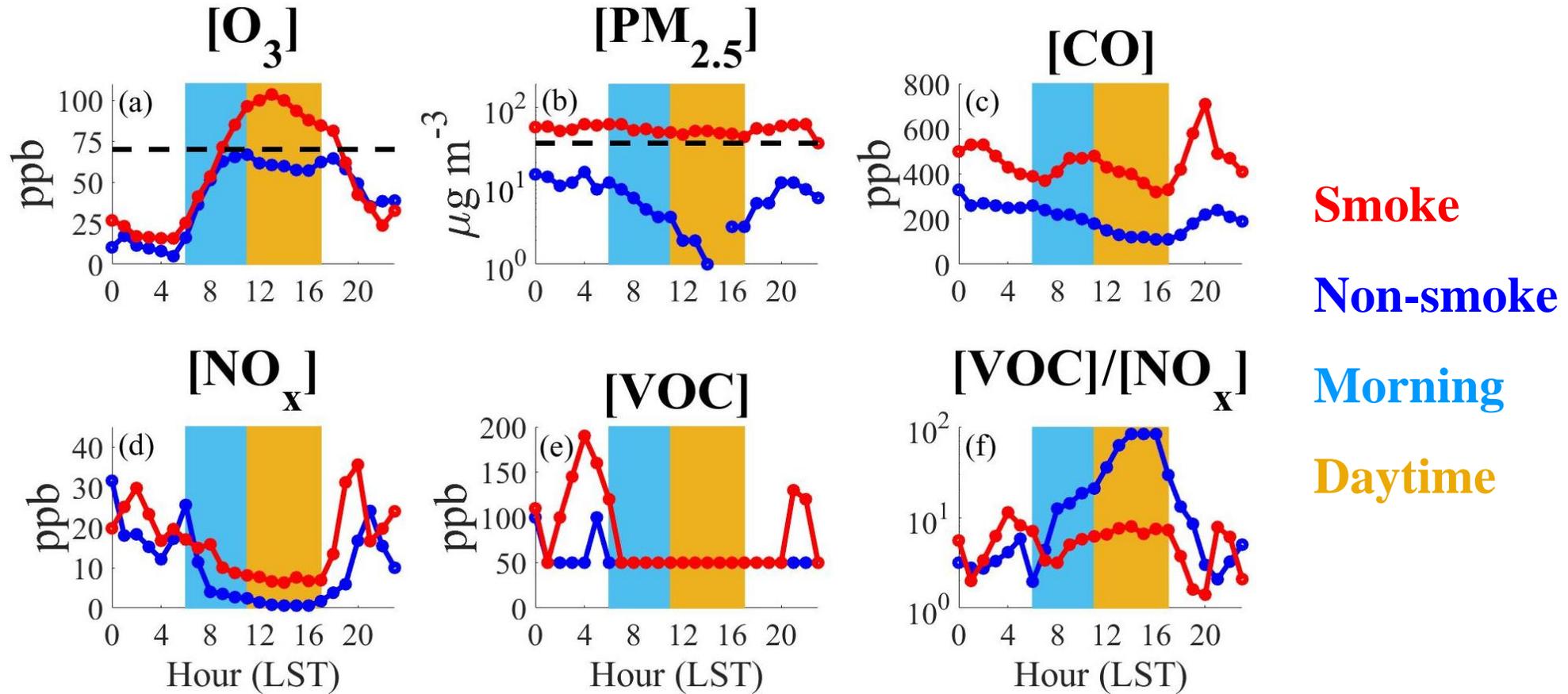
## Key assumptions made regarding initial conditions:

1. Assumed concentrations of unmeasured chemical species that influence  $O_3$  formation chemistry (e.g., peroxyacetyl nitrate (**PAN**), nitric acid (**HNO<sub>3</sub>**), nitrous acid (**HONO**), etc.)
2. Assumed concentrations of unmeasured radical species that initiate and/or propagate  $O_3$  formation process (e.g., hydroxyl radical (**OH**), organic peroxy radicals (**R<sub>i</sub>O<sub>2</sub>**), etc.)
3. Speciated VOC data = daily-averaged
  - Speciated VOC concentrations (**[VOC<sub>i</sub>]**) were scaled to match hour-averaged total [VOC]

## Other details regarding F0AM:

- Version 3.3.1 of the Master Chemical Mechanism (**MCM**; <http://mcm.leeds.ac.uk/MCM>) was used to drive the model chemistry
- Background concentrations of O<sub>3</sub>, CO, and 7 VOCs (acetaldehyde, acetone, ethane, formaldehyde, isopentane, n-butane, and propane) were included
  - **Collectively:** the 7 above VOCs comprised ~80% of [ΣVOC<sub>i</sub>] for the **smoke** and **non-smoke** cases
- F0AM-predicted total [NO<sub>x</sub>] was scaled to constraints – important to note that NO and NO<sub>2</sub> were still allowed to vary throughout the model simulations
- 24-hour simulations were conducted for the **smoke** and **non-smoke** cases, with a 2-day model spin-up and a 10-minute integration time for each model time step

# Observed concentrations for **smoke** and **non-smoke** days



- Note log scale for [PM<sub>2.5</sub>] and [VOC]/[NO<sub>x</sub>] figures
- Precision issue regarding total [VOC] measurements? **(more on this later)**

# Results – F0AM predictions

## To reiterate:

- Our objective is to use F0AM to investigate smoke impacts on  $O_3$

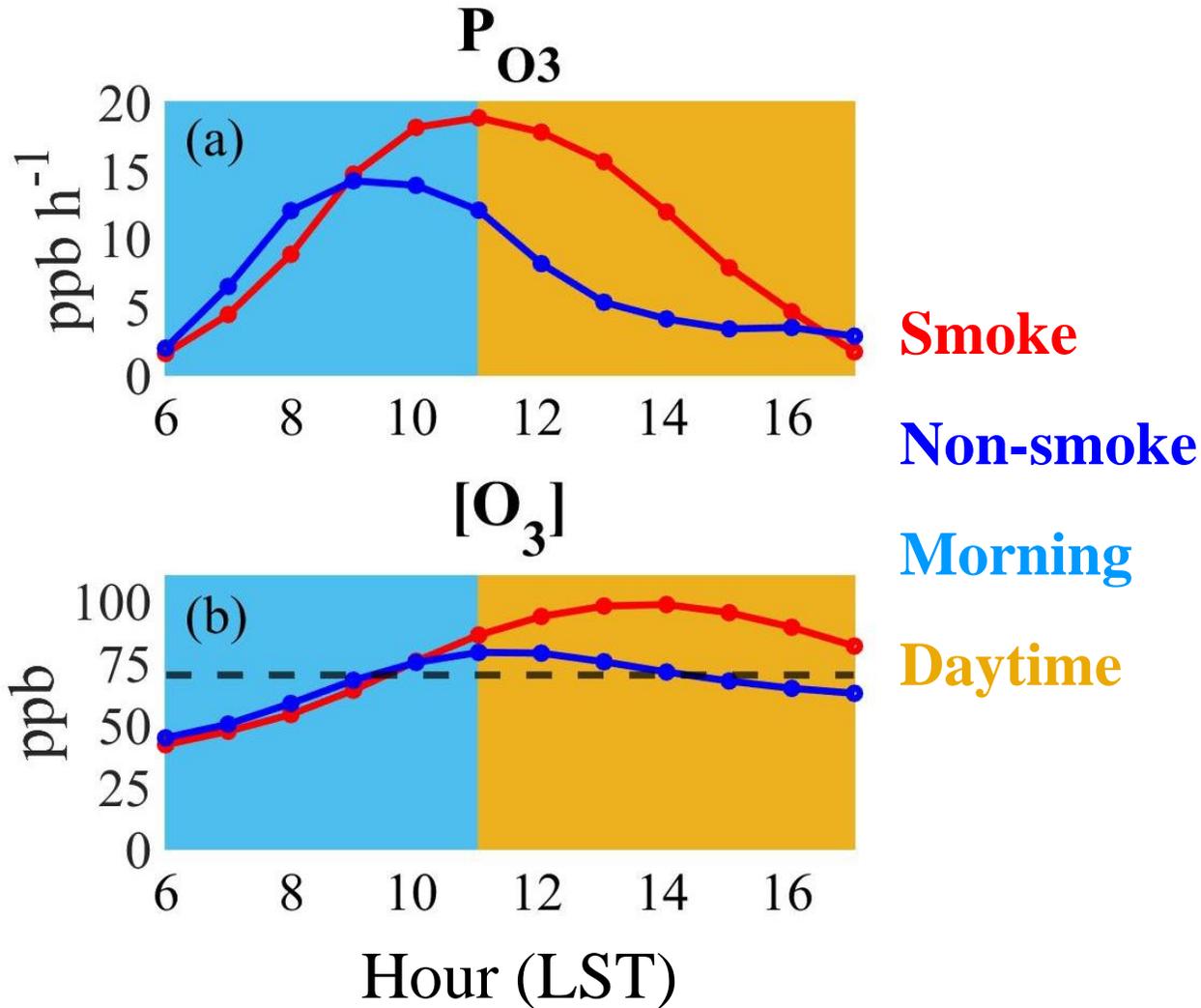
## As a result:

1. We compared the F0AM-predicted  $O_3$  production rate ( $P_{O_3}$ ) and  $[O_3]$  for the **smoke case** versus the **non-smoke case**

$P_{O_3}$  = the sum of the  $HO_2 + NO$  and  $R_iO_2 + NO$  reaction rates

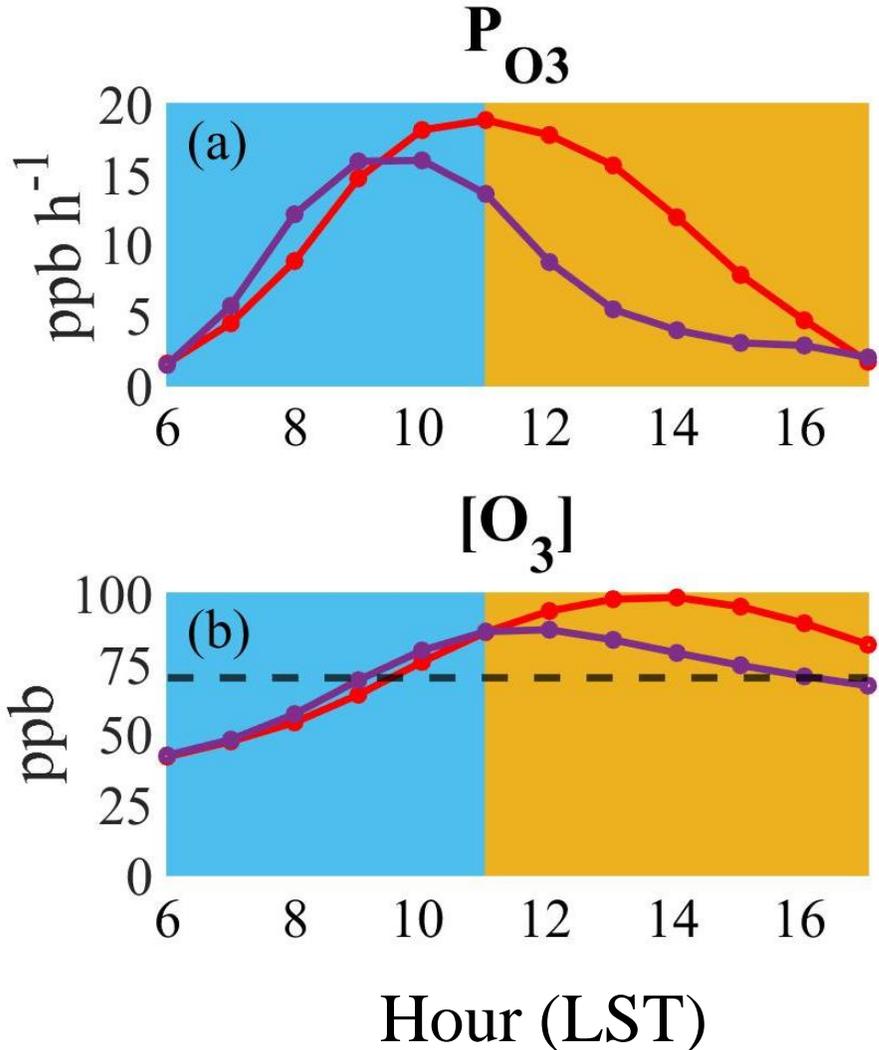
- $R_iO_2$  accounted for methylperoxy, ethylperoxy, acetylperoxy, and acetonylperoxy radicals, each of which were initialized in F0AM
2.  $[NO_x]$  on the **smoke day** was set equal to  $[NO_x]$  on the **non-smoke day** to examine the extent to which the higher  $[O_3]$  on the **smoke day** may have been affected by higher daytime  $[NO_x]$

# (1) FOAM $P_{O_3}$ and $[O_3]$



Comparison of the FOAM-predicted  $O_3$  production rate ( $P_{O_3}$ ) and  $[O_3]$  for the smoke case versus the non-smoke case

# (2) How does $\text{NO}_x$ impact the $\text{O}_3$ production on the **smoke** day?



**Initial results**

$$\text{NO}_{x, \text{smoke}} = \text{NO}_{x, \text{non-smoke}}$$

**Morning**

**Daytime**

- **To examine the above question:** observed  $[\text{NO}_x]$  on the **smoke day** was changed to equal observed  $[\text{NO}_x]$  on the **non-smoke day**
- Results suggest that the  $\text{O}_3$  production regime =  **$\text{NO}_x$ -sensitive**

## Summary:

- Daytime  $P_{O_3}$  = up to  $\sim 10$  ppb  $h^{-1}$  **greater** during the **smoke case**, consistent with the enhanced model-predicted and observed  $[O_3]$
- Model sensitivity test results indicate that the elevated daytime  $[O_3]$  on the **smoke day** was influenced by daytime  $[NO_x]$  being  $\sim$  an order of magnitude greater compared to the **non-smoke day**
  - $O_3$  production regime = likely  **$NO_x$ -sensitive**

## Next steps:

1. Conduct additional sensitivity studies to further assess the impact of  $[VOC_i]$  and  $[NO_x]$  on  $P_{O_3}$  and  $[O_3]$  during the **smoke case**

## Next steps continued

2. Address potential precision issue regarding total [VOC] measurements
  - Total [VOC] reported in units of ppm (to 2 decimal places)
  - Higher [PM<sub>2.5</sub>] and [CO] during the **smoke case** indicate that [VOC] should be higher on the **smoke day** compared to the **non-smoke day**
  - **However:** measurements suggest that total [VOC] = a constant 50 ppb for most of the day on the **smoke and non-smoke** cases
  - **Consequently:** we plan to scale [VOC<sub>i</sub>] to [CO], which will approximately **double** the [VOC<sub>i</sub>] specified in FOAM on the **smoke day**
  - This should further increase the sensitivity of O<sub>3</sub> to NO<sub>x</sub> during the **smoke case**
3. Apply a similar methodology to study the impact of wildfire smoke on O<sub>3</sub> for other U.S. cities

**\*\* This is a work in progress, so comments and suggestions are welcome! \*\***

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