Using Photochemical Models to Assess the Exceptional Event Rule's Q/D Screening Guidance

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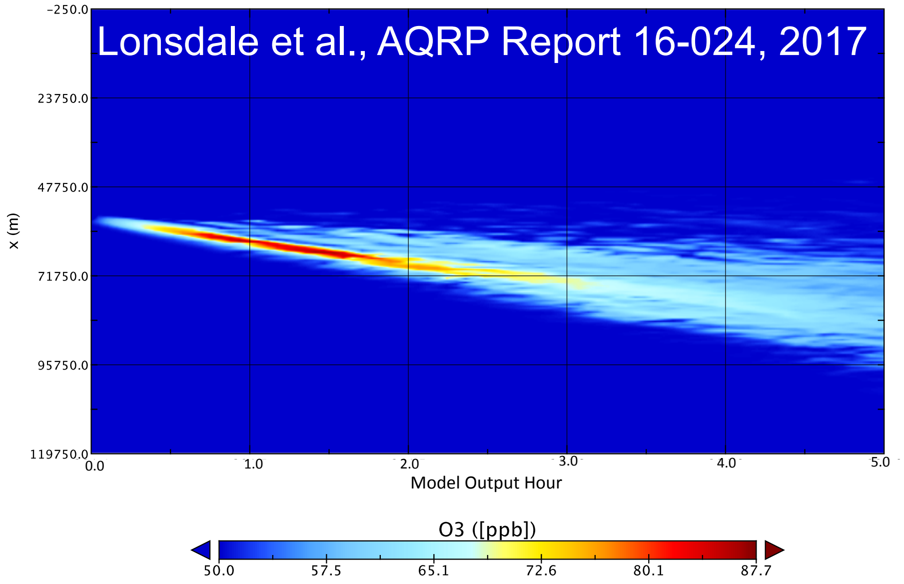
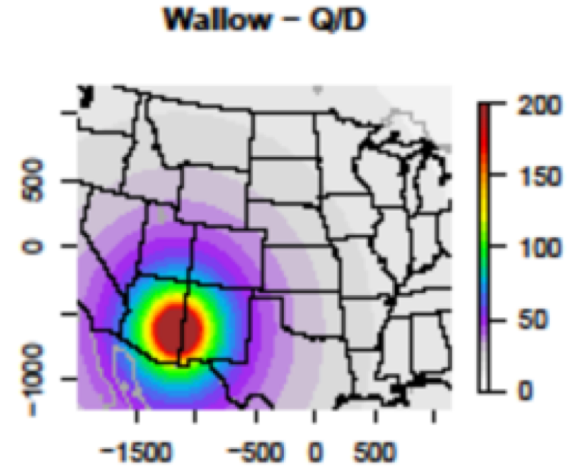
Wildfire Exceptional Event Demonstrations

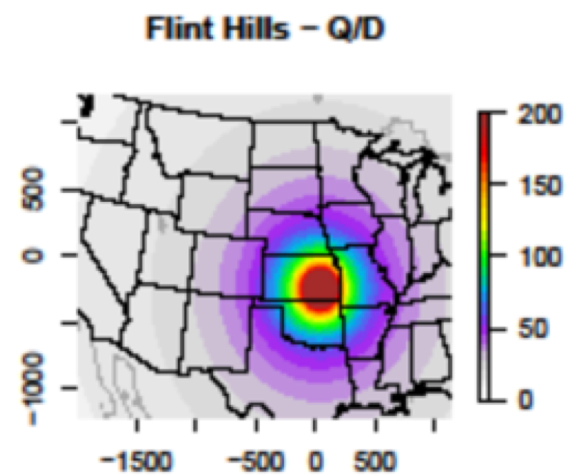
- Poor air quality events due to wildfires can be excluded from NAAQS attainment.
- Must demonstrate a ***clear, causal relationship*** between the wildfire event and the monitor.
- Photochemical models can be used to calculate the O_3 impacts of fires, but they are computationally expensive.
- ***Thus, there is a need for screening methods to identify likely exceptional events.***



Screening Wildfire Impacts of Ozone

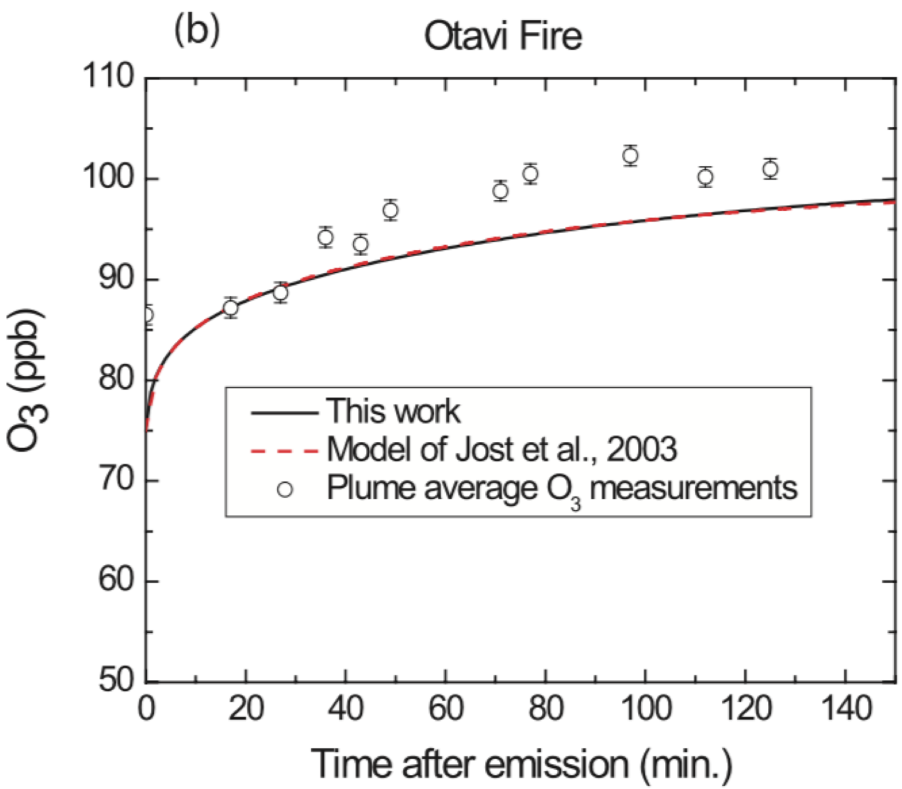
- 'Q/D' Metric
  - Q : NO_x and VOC emissions from fire
  - D : Distance of monitor from fire
  - If Q/D > 100 tons/day/km, no photochemical modeling (Tier 2)
- EPA notes that:
  - Q/D alone is not enough to demonstrate O_3 impacts
  - Threshold of 100 tpd/km is a "conservative value"





Is the Q/D metric appropriate for O_3?

- O_3 is a secondary pollutant rapidly produced by the photochemistry of NO_x and VOCs emitted by fires
- **The concentration of O_3 *increases* with distance downwind** until plume dilution is greater than chemical production



Alvarado and Prinn., JGR, 2009

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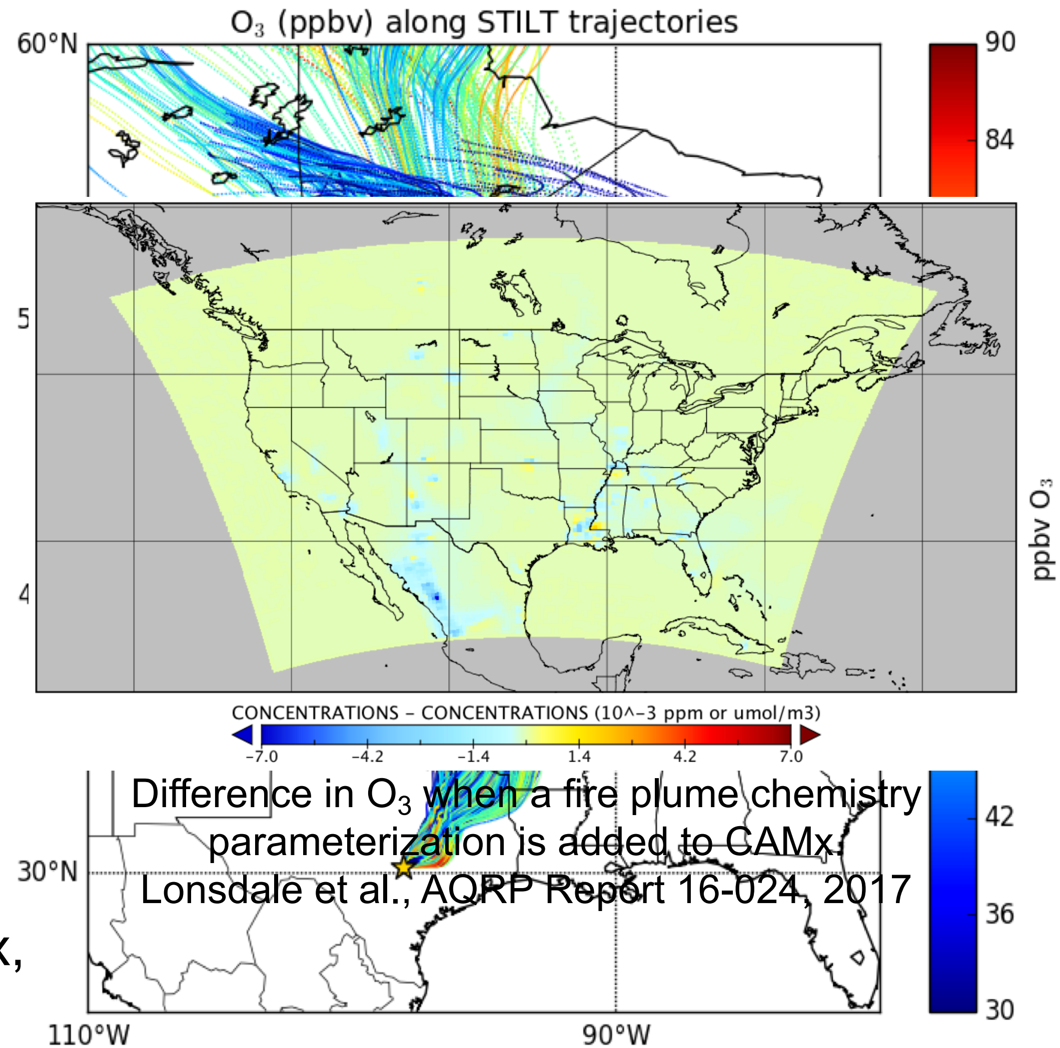
Investigating the Q/D Metric for Wildfires

- Literature Review
- Simulate two Texas fire events
  - El Paso event from Hog Fire
  - Houston event from Yucatan
- Using three photochemical modeling approaches
  - Lagrangian parcel model (ASP)
  - Lagrangian chemical transport model (STILT-ASP)
  - Eulerian grid model (CAMx, El Paso only)



Difference in O_3 when a fire plume chemistry parameterization is added to CAMx.
Lonsdale et al., AQRP Report 16-024, 2017

Lonsdale et al., AQRP Report 16-024, 2017

Literature summary of Q/D versus O_3

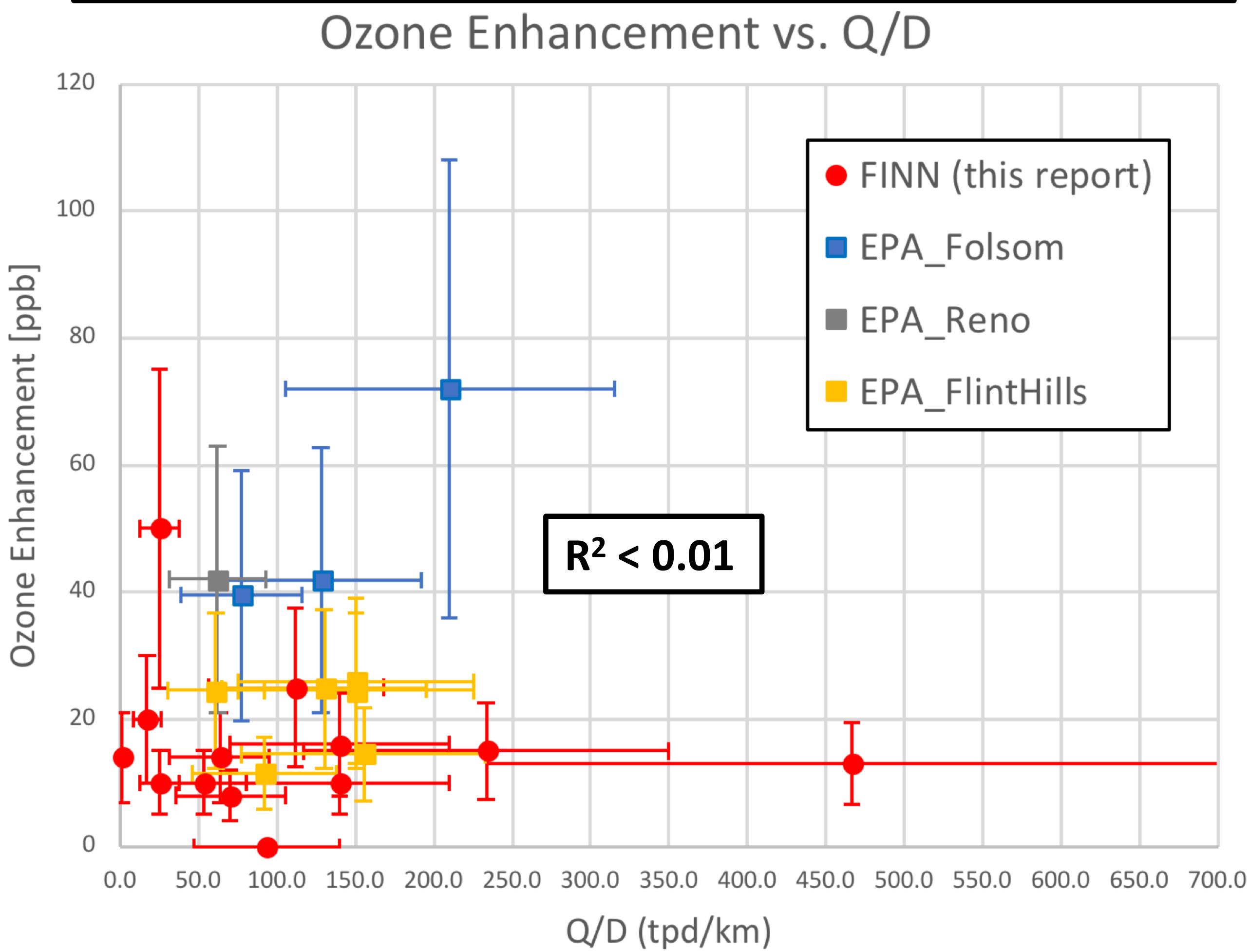
Location	Q [tpd]	D [km]	Q/D [tpd/km]	O_3 Enhancement	Citation
Wallow	6,000	350	17.1	20	Baker et al. 2016
Flint Hills	28,000	250	112.0	25	Baker et al. 2016
Mexico City	14,000	150	93.3	0	Lei et al., 2013
Western Canada	80,000	1,500	53.3	10	Lindaas et al, 2017
Western US	34,000	1,350	25.2	10	Lindaas et al., 2017
Maryland	1,500	1,700	1.0	14	Dreessen et al., 2016
Western US	70,000	1,100	63.6	14	Gong et al. 2017
Western US	70,000	1,000	70.0	8	Gong et al. 2017
Western US	70,000	500	140.0	16	Gong et al. 2017
Western US	70,000	500	140.0	10	Gong et al. 2017
Western US	70,000	300	233.3	15	Gong et al. 2017
Western US	70,000	150	466.7	13	Gong et al. 2017
Alaska and Canada	100,000	4,000	25.0	50	Morris et al., 2006

NOTES: Alaska and Canada Q estimate very approximate, see Turquety et al. (2007)

Baker et al. (2016) D values are from fire centroids and nearest point in Texas

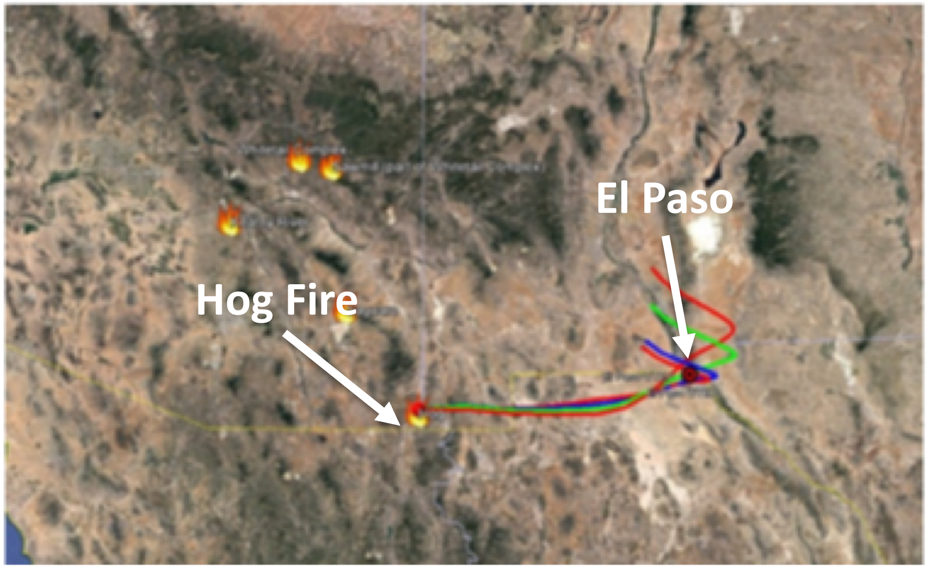
O_3 enhancement not a function of Q/D

O_3 Enhancement (ΔO_3) = O_3(in plume) – O_3 (background)



El Paso Case Study – Hog Fire

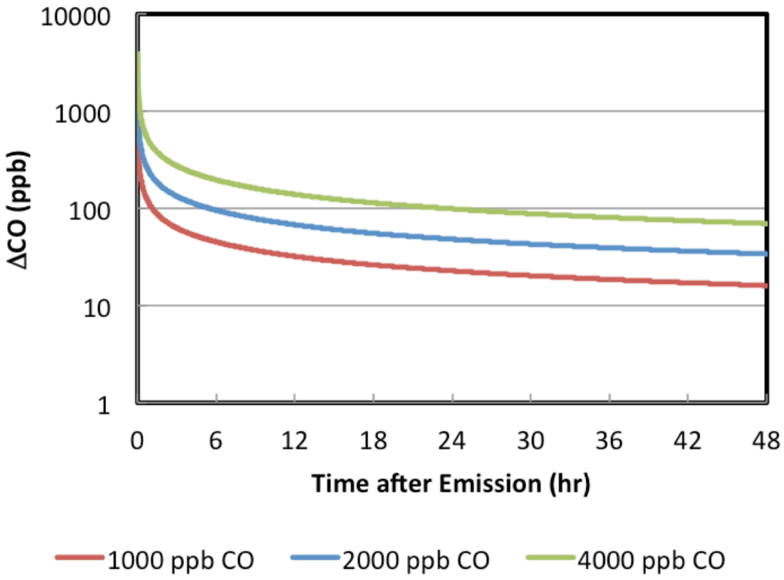
HYSPLIT Back-Trajectories for CAMS 12.

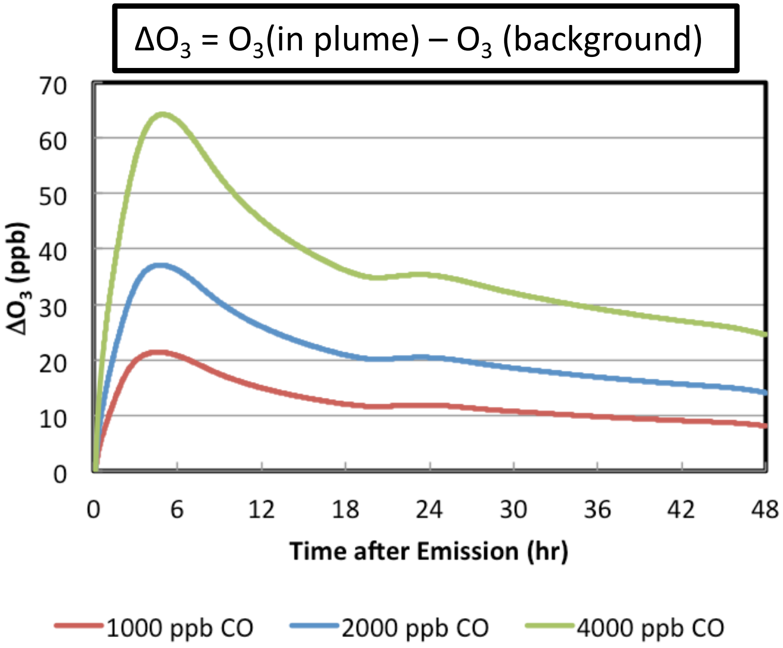


HYSPLIT Forward Trajectories from Hog Fire.

	VOC [tpd]	NOx [tpd]	Q [tpd]	2-day Q [tpd]	D [km]	Q/D, 1-day [tpd/km]	Q/D, 2-day [tpd/km]
21-Jun	89	7	96	188	250	0.384	0.752
20-Jun	85	7	92	176	250	0.368	0.704
19-Jun	78	6	84	195	250	0.336	0.78
18-Jun	103	8	111	173	250	0.444	0.692
17-Jun	57	5	62	94	250	0.248	0.376
16-Jun	30	2	32		250	0.128	

Hog Fire Lagrangian Parcel Simulations





- O_3 enhancement increases for first 6 hours after emission (if emitted at 12:00 LST), then decreases, which is not consistent with Q/D
- O_3 enhancement is roughly proportional to initial plume concentrations
  - Initial concentration controlled partly by emissions (Q), but also mixing height, fire size, wind speed, etc.

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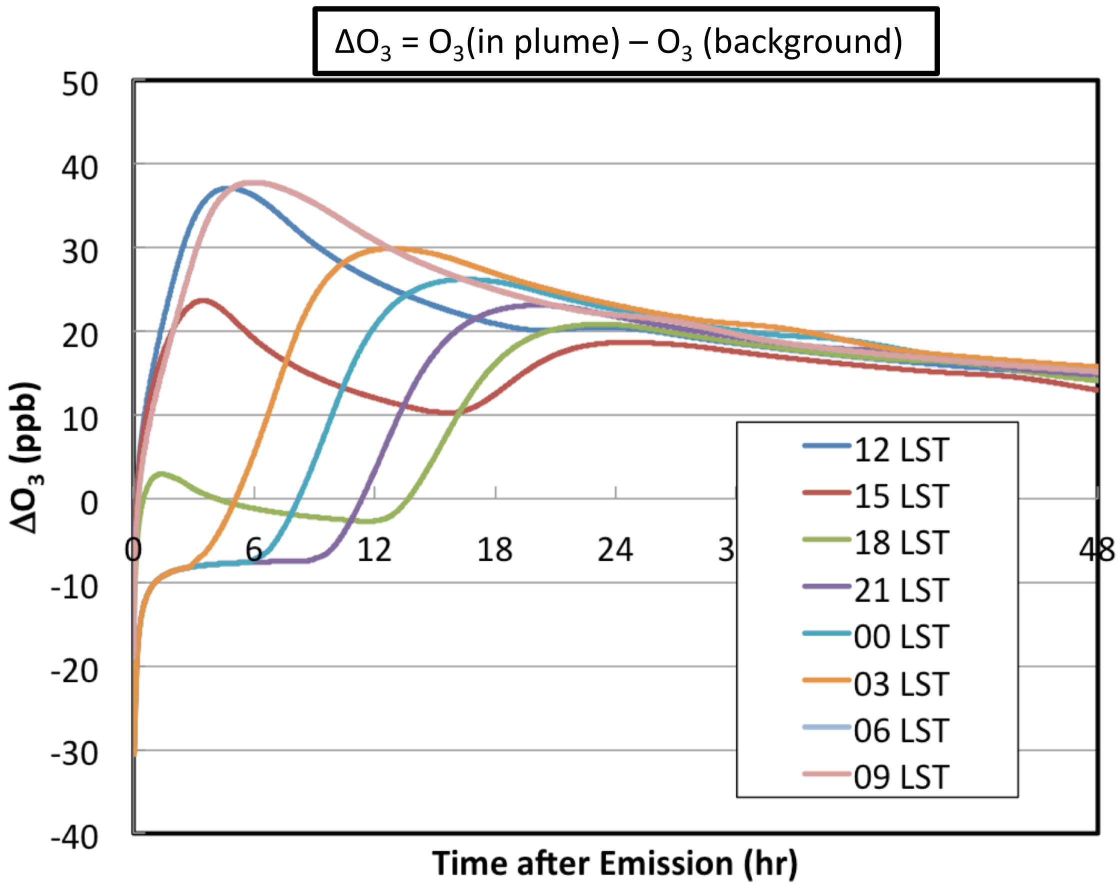
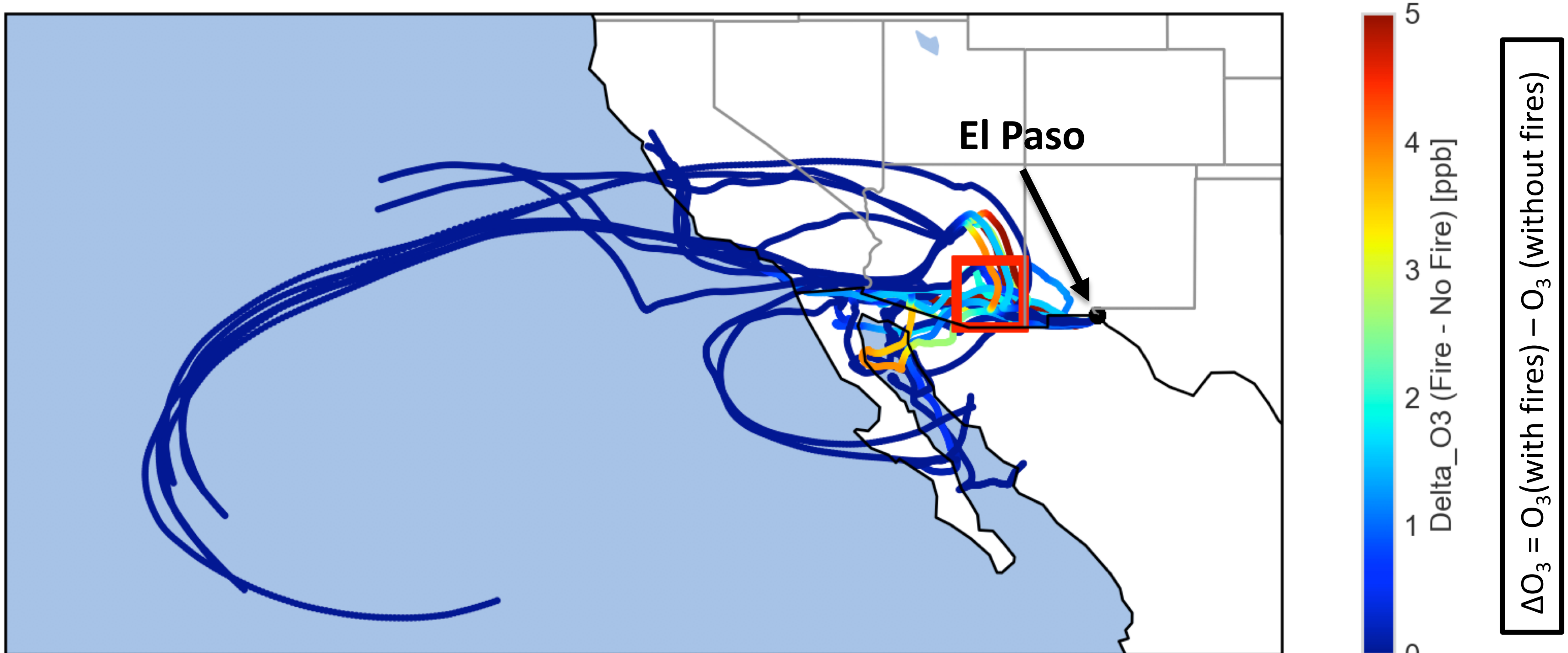
Hog Fire Lagrangian Parcel Simulations

- O_3 enhancement in first 24 hours depends on what time of day the parcel is emitted, but **enhancements all very similar after 24 hours**!
- Consistent with review of Jaffe and Wigdar (2012), which suggested similar values for $\Delta O_3/\Delta CO$ after 1-2 days aging.

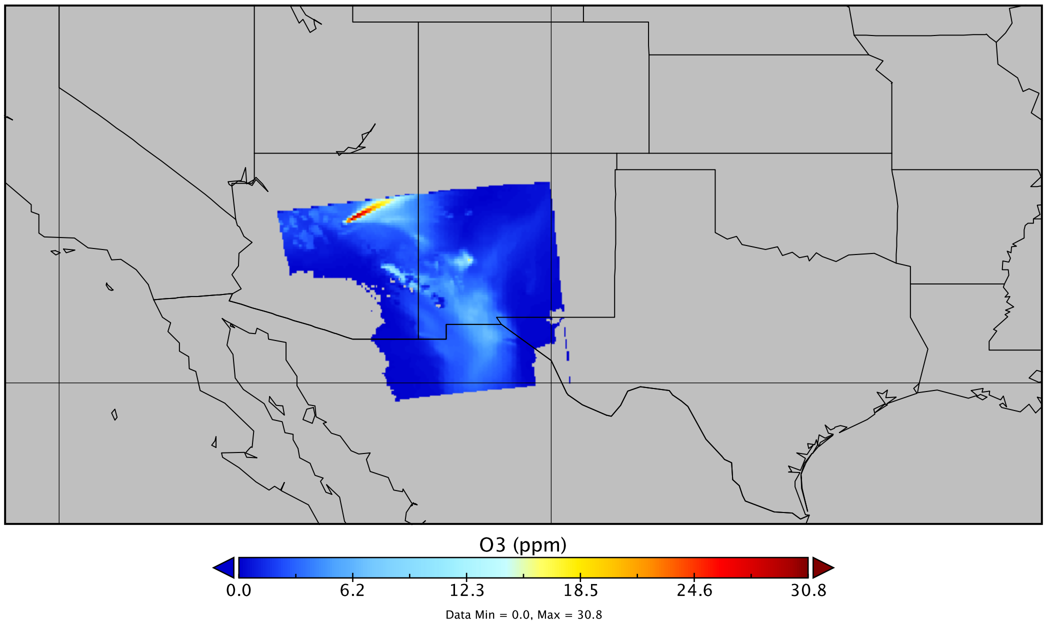


El Paso Lagrangian CTM Simulations



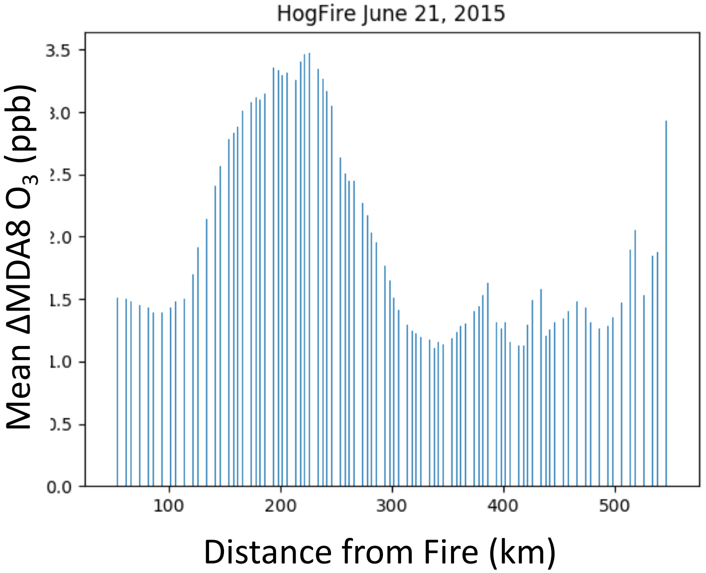
- Only small fraction of the 500 back-trajectories encountered the fires.
- O_3 enhancement is produced near the fire source and stays constant with distance after that.
- "Straight line" distance a poor proxy for trajectory distance or parcel age.

El Paso CAMx simulations (Performed by Ramboll, provided by TCEQ)



Difference in MDA8 O_3 due to fire emissions.

$\Delta O_3 = O_3(\text{with fires}) - O_3\ (\text{without fires})$



Average difference in MDA8 O_3 with distance from the Hog Fire.

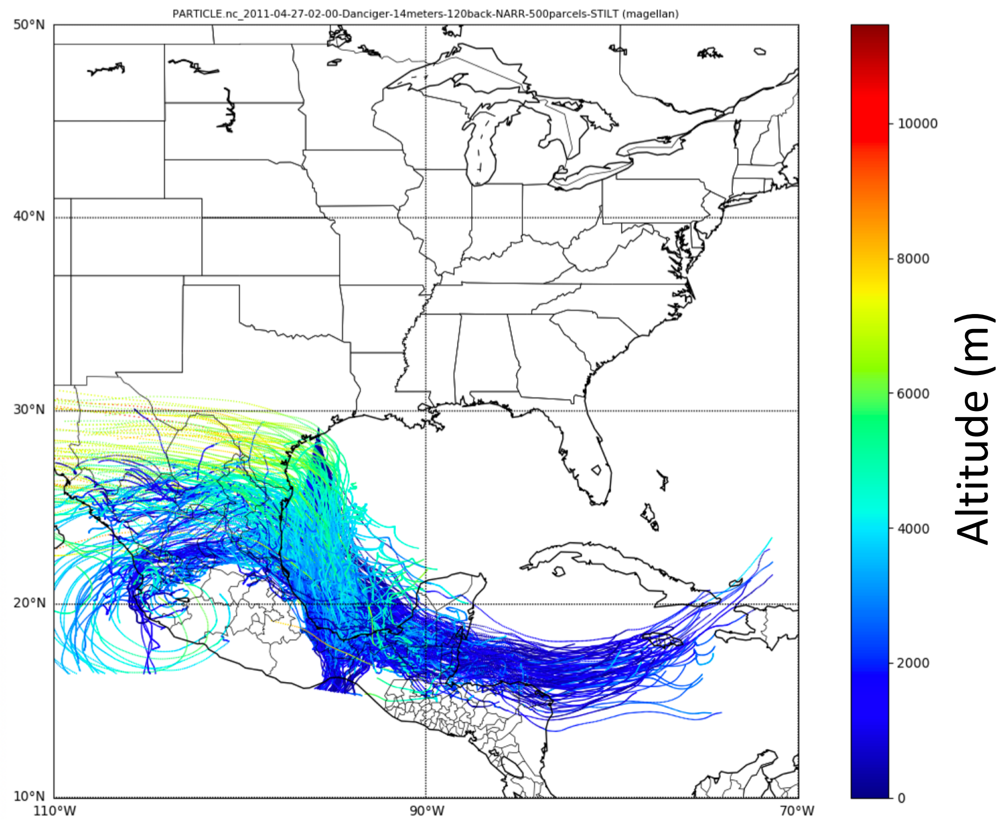
MDA8 O_3 impact increases with distance from fire up to ~225 km. Inconsistent with Q/D, but consistent with Lagrangian parcel simulations.

Houston Case Study – Yucatan Fires

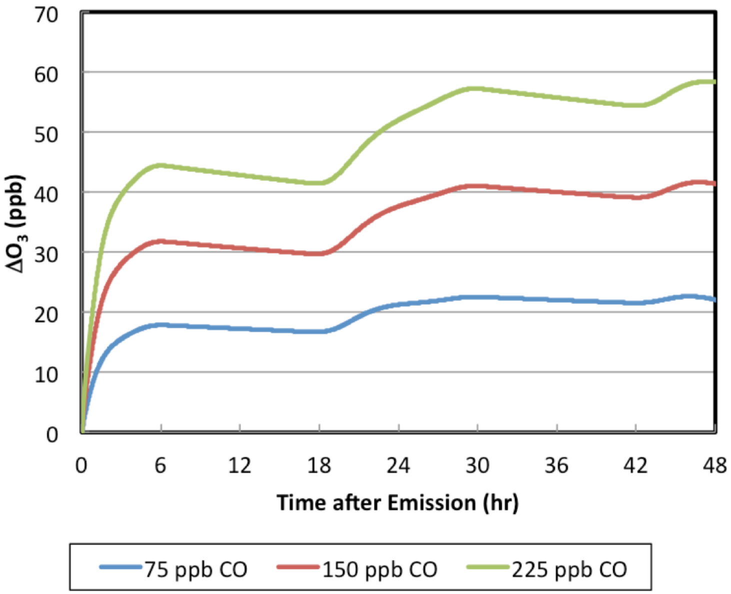
- Two events identified by Prof. Yuxuan Wang of the University of Houston.
  - April 26-27, 2011
  - May 1-2, 2013

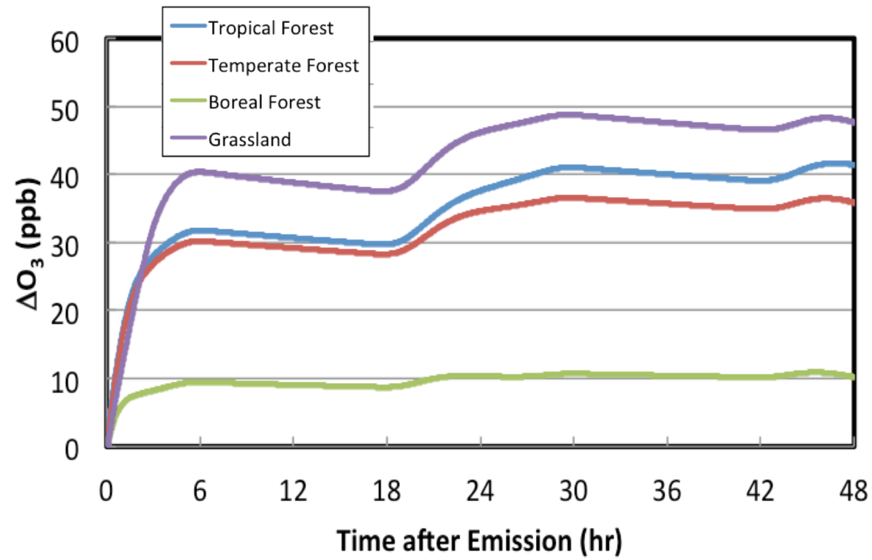
	Q [tpd]	D [km]	Q/D [tpd/km]
26-Apr-11	158,800	1,000	159
27-Apr-11	265,000	1,000	265
30-Apr-13	140,000	1,000	140
1-May-13	157,000	1,000	157
2-May-13	244,000	1,000	244

April 26, 2011



Houston Lagrangian Parcel Simulations

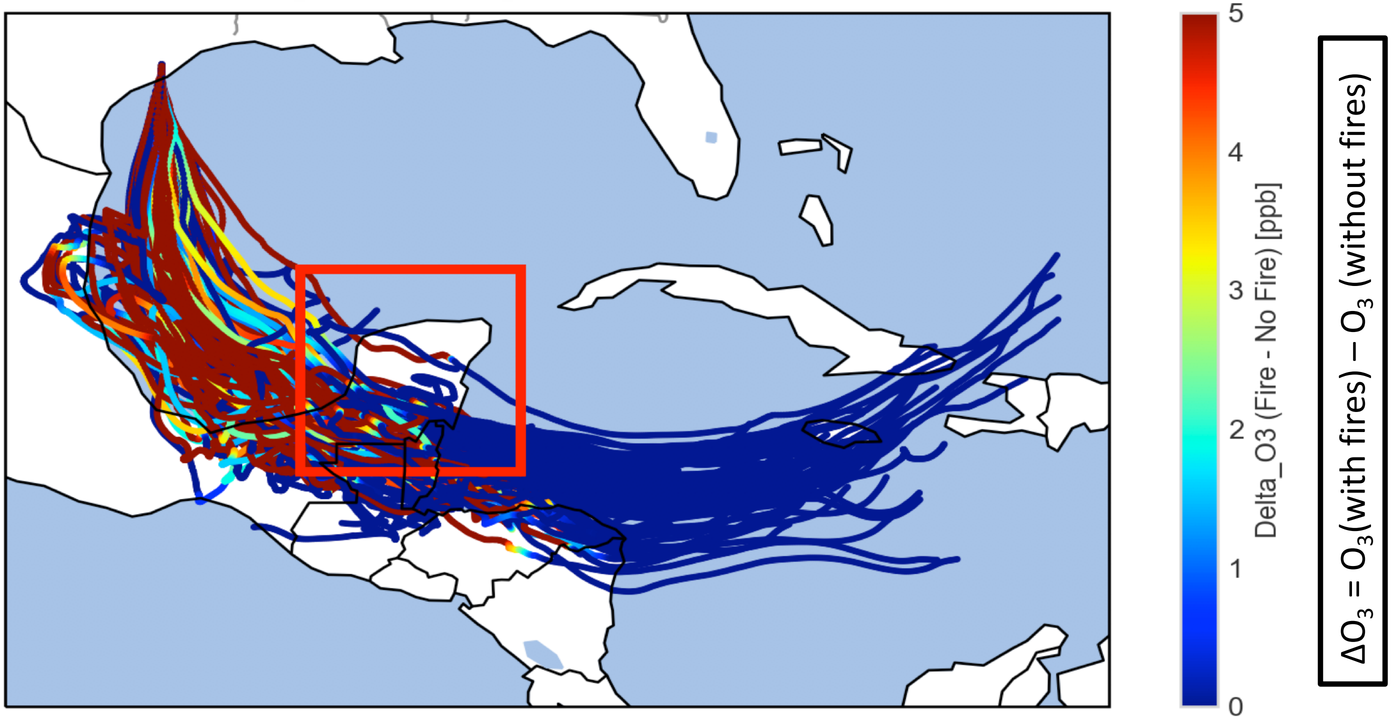




- Yucatan plume is large, so dilution is very slow
- O_3 increases for at least 2 days
- O_3 enhancement proportional to initial plume concentrations, consistent with Q/D if all else is equal (e.g., PBL height)

- Tropical forest, temperate forest, and grassland emission factors all have similar changes in O_3 enhancement with time after emission (and thus distance)
- But **boreal forests make much less O_3 for same Q (NO_x+VOCs)** suggesting they need a different Q/D threshold.

Houston Lagrangian CTM Simulations



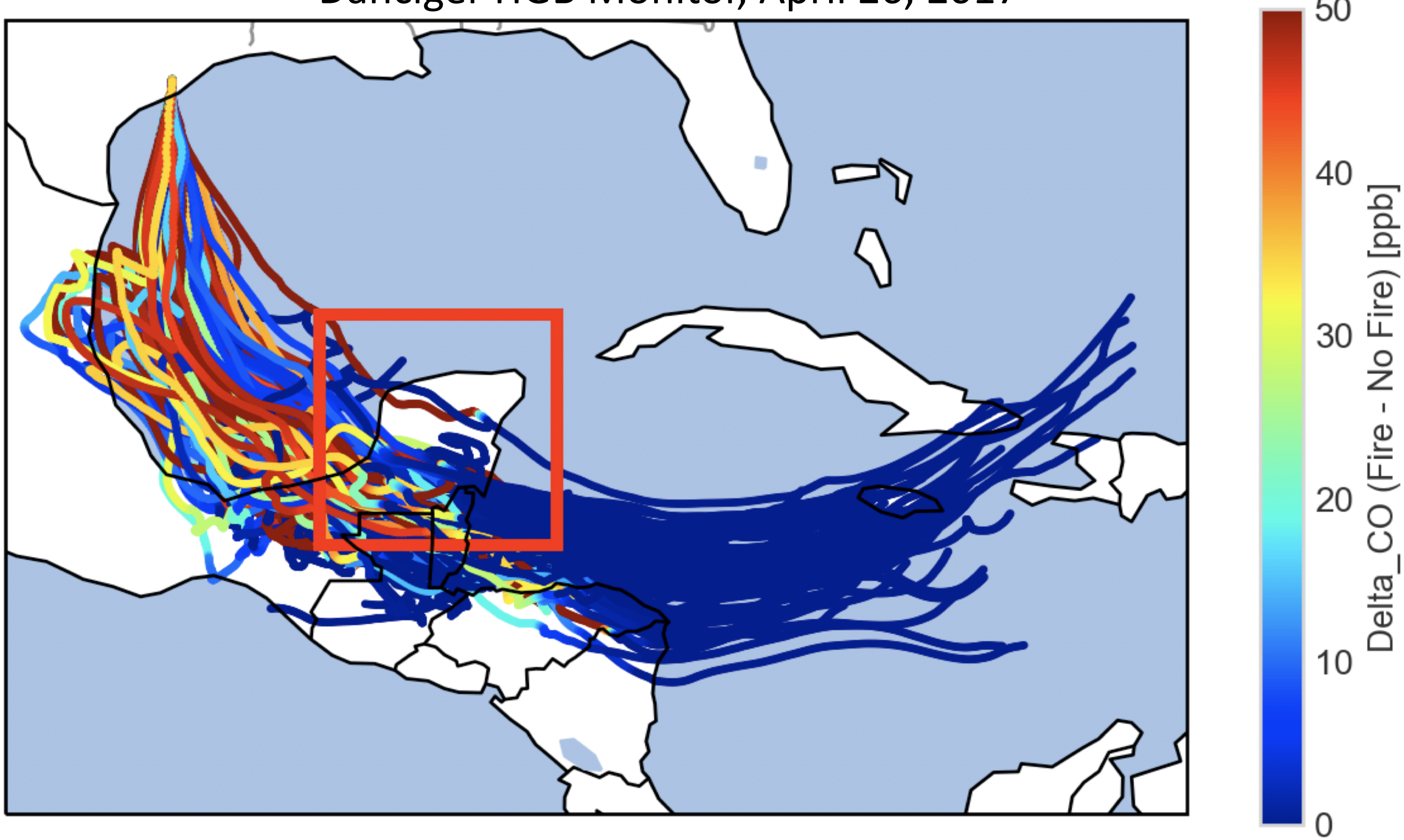
- About a third of the 500 back-trajectories encountered the fires.
- O_3 enhancement is produced near the fire source, increases for some distance downwind, then decreases.

Alternative Screening Metrics

- **Use Jaffe and Wigder (2012) review as the basis of a screening metric.**
  - $\Delta O_3/\Delta CO = 0.2 \pm 0.1$ after 1-2 days (-0.1 to 0.9)
  - Boreal forest lower, $\Delta O_3/\Delta CO = 0.005 \pm 0.019$ (Alvarado et al., 2010)
- **Use STILT or HYSPLIT back-trajectories and fire CO emission inventories to estimate ΔCO.**
  - Could use $\Delta O_3/\Delta NO_y$ or $\Delta O_3/(\Delta NO_y+VOCs)$ instead

Alternative Screening Metrics

Danciger HGB Monitor, April 26, 2017



Example: ΔCO is ~20 ppbv from STILT, so we expect **2-6 ppbv O_3** from the fires. Full STILT-ASP simulation gave 1.8 ppbv, but this may be an underestimate due uncertain organic nitrate chemistry (Lonsdale et al., 2017).

Conclusions

- **The Q/D metric is not consistent with the literature or the photochemical modeling performed in this study.**
  - The Lagrangian parcel (ASP) simulations show O_3 increasing with distance downwind.
    - The O_3 was proportional to Q if other parameters (e.g., mixing height, fire area) are held constant.
    - O_3 formation from boreal forest fires is lower than other fuel types.
  - The meandering STILT-ASP trajectories suggest straight-line distance is a poor proxy for parcel age or dilution rate.
  - CAMx-simulated fire impacts on MDA8 O_3 for the El Paso event increase with distance within 200 km of the fire.
- **We recommend an approach that uses literature values of ratios of $\Delta O_3/\Delta CO$ or $\Delta O_3/\Delta NO_y$ with STILT and HYSPLIT back-trajectories.**