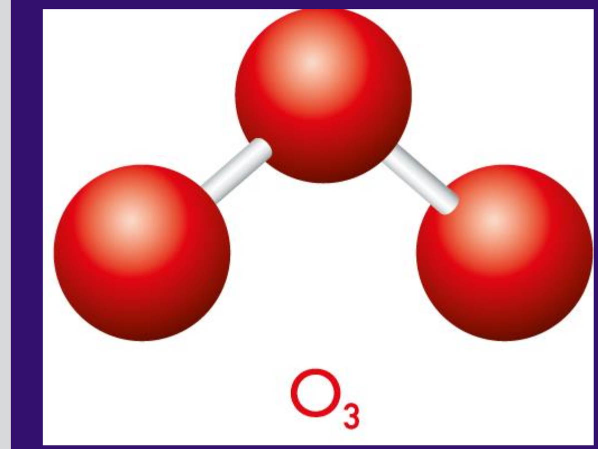

Understanding O_3 dynamics with TEMPO observations in Salt Lake City and Nationally

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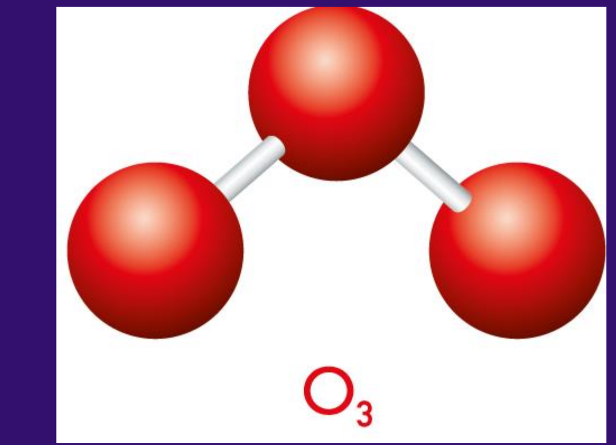

Project 1 (funded): VOC to NOx relationships and Impacts of Smoke on Ozone in the Salt Lake City, UT region.

The Salt Lake metropolitan region is one of about 50 regions in the U.S. that do not meet the 2015 O_3 standard (annual fourth highest maximum daily 8-hour average (MDA8, averaged over three years). Local emissions from vehicles and industry make a significant contribution to this O_3, but so do background sources including wildfires. In this project we will look at both the controllable (local) sources of O_3 along with the contribution from wildfire smoke.

The figure below shows the annual fourth highest MDA8 at one site in SLC (Hawthorne) for 2000-2023. Despite significant emission reductions, there has been change in the fourth highest O_3 value. High fire years show especially high O_3 values. But even in low fire years (like 2019) SLC still exceeds a 70 ppb level. Controlling the local emissions further should help. Our project is intended to examine the VOC vs NOx sensitivity using both surface observations and satellite TEMPO and TROPOMI data and this can provide useful information on the most efficient way to reduce O_3 in the region.

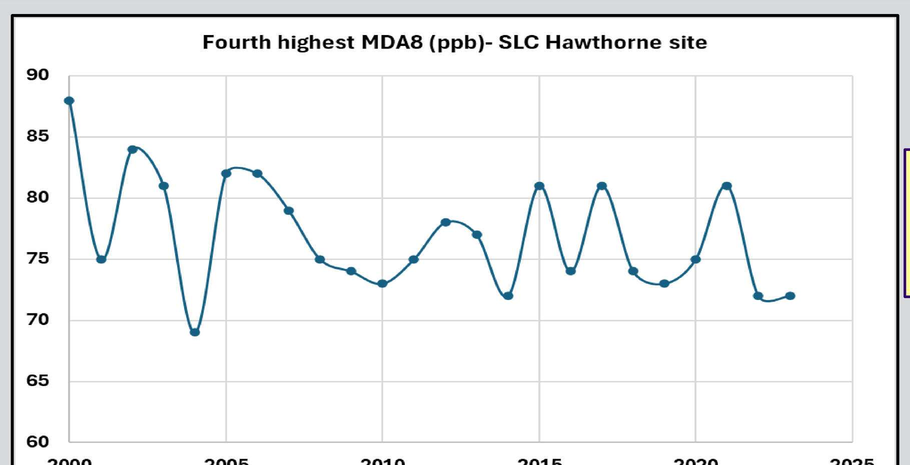

Figure 1: Annual fourth highest MDA8 as measured at the downtown Hawthorne site in SLC.

Previous work in SLC

In the summer of 2022, at team from UW, U-Montana and Utah State U completed the Salt Lake Regional Smoke, Ozone, and Aerosol study (SAMOZA) . This project conducted in-situ observations of O_3, NOx, CO and a suite of VOCs by PTR-MS. Formaldehyde was measured by two separate methods. The observations took place at the Utah Tech Center, which is near the city core. Photochemical modeling (using the FOAM box model) and statistical modeling (GAMs) were also completed. The photochemical modeling and the observed FNR present a consistent picture of VOC sensitivity. Figure 2 shows a strong VOC sensitivity to O_3 production from the modeling. In contrast to the VOCs, large reductions are NOx are needed before the O_3 production rates are significantly reduced. Figure 3 shows the observed FNR on both exceedance days (MDA8> 70 ppb) and non-exceedance days. For all hours of the day, the FNR is well below the transitional threshold (ca 3), indicating VOC sensitivity. So both the modeling and observed FNR paint a consistent picture of VOC sensitivity at the downtown UTC site.

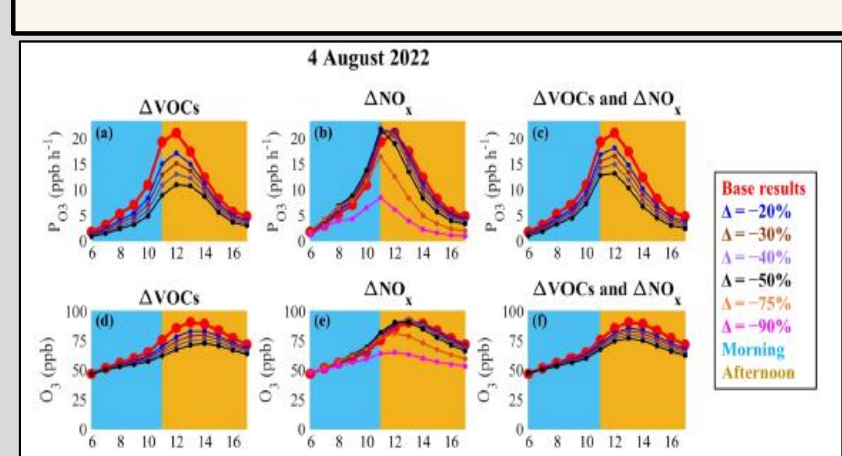

Figure 2. Photochemical modeling using SAMOZA data on a non-smoky high O_3 day. The strong sensitivity of O_3 production to VOCs and less sensitivity to NOx indicate a "VOC sensitive" regime. (Ninneman et al 2023)

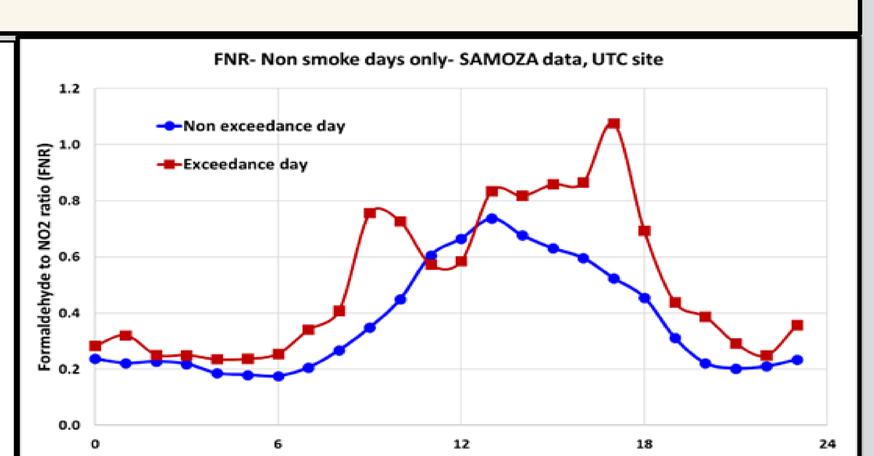

Figure 3. Formaldehyde to NO_2 ratio observed on non-smoke days in August-September 2022. This include 3 exceedance days (MDA8>70 ppb) and 48 non-exceedance days. (Jaffe et al 2024)

The Formaldehyde to NO_2 Ratio

Formaldehyde and NO_2 are key precursors and intermediates in the photochemical production of O_3. We have previously measured both compounds at the surface. Both formaldehyde and NO_2 are clearly observed by space based instruments and the FNR from satellite observations is a good indicator of the VOC vs NOx sensitivity for O_3 production (Souri et al 2020; Tao et al 2022; Jin et al 2023). An FNR value of <3 is consistent with a VOC sensitive O_3 production regime whereas values >3 are consistent with a NOx sensitive regime (Jin et al 2020; Tao et al 2022).

The Formaldehyde to NO_2 Ratio: What really matters?

We often treat O_3 production as a static process. By this I mean, we assume that only the <u>local</u> NOx and VOCs control the process. But O_3 production occurs over (roughly) an 8-hour time frame during the day and during this time, an air mass can easily move over 100 km. So what really matters is the VOC to NOx sensitivity over the entire period of O_3 production as an airmass moves (in other words, the integrated O_3 production). This is where TEMPO data will provide an extraordinary view of the relevant parameters.

Figure 4 shows a one month average of the FNR over northern Utah from the TROPOMI instrument. Higher values are seen in the urban/SLC area and lower values elsewhere. Also shown are one month of 24-hour backward trajectories. This supports the point above: that the O_3 production regime must take into account the VOC and NOx concentrations during the previous day.

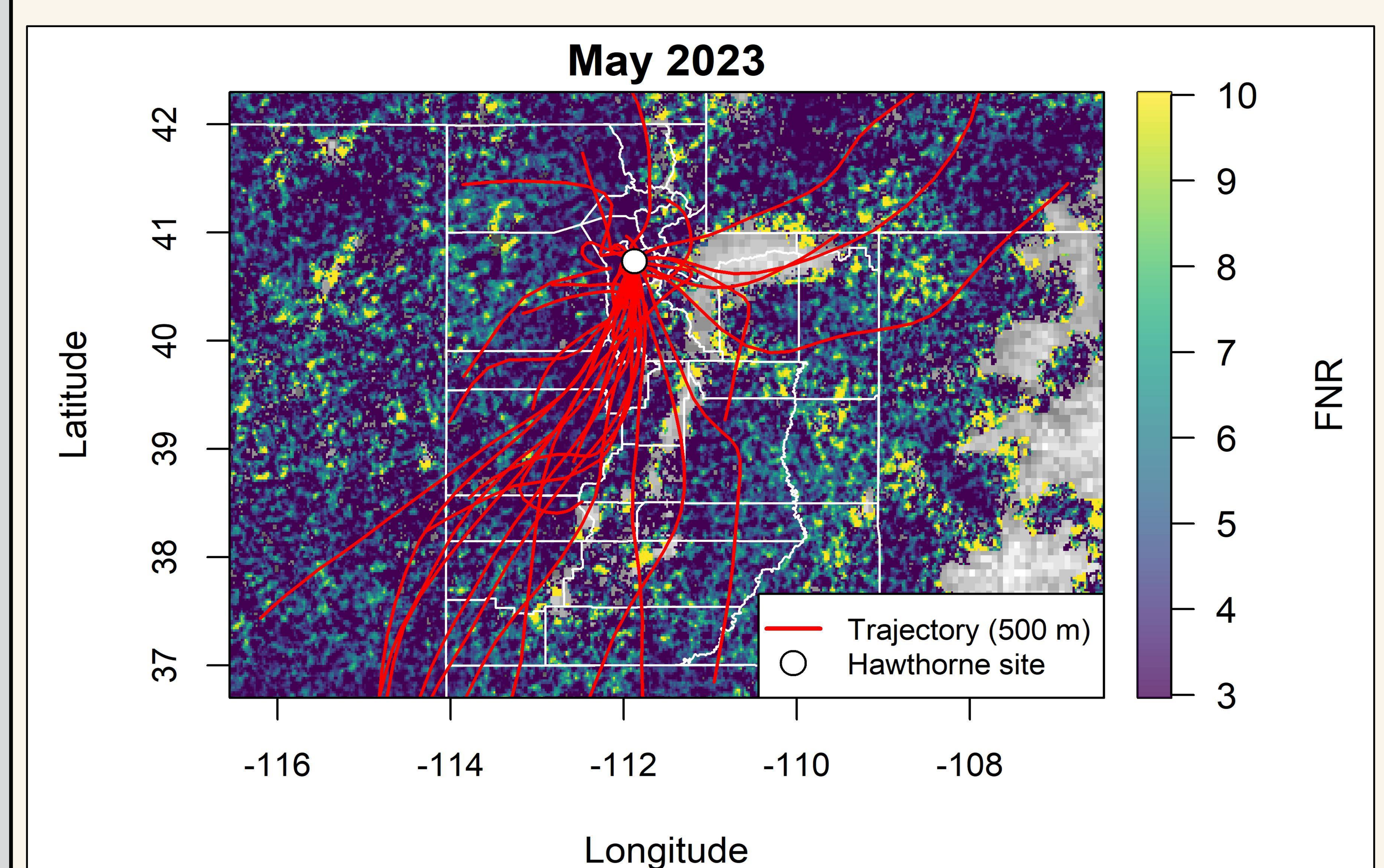

Figure 4. TROPOMI FNR for May 2023 over northern Utah overlaid with 24-hour back trajectories. Initialized from the Hawthorne monitoring site in SLC.

Project 2: (Proposed): Hindcast predictions of O_3 using satellite NO_3 and CH_2O in a machine learning framework.

We have proposed to build on our existing machine learning/Generalized Additive Modeling approach for hindcasting surface O_3 at all US regulatory air quality stations. This method also can quantify the smoke contribution to surface O_3 on every day with smoke. Shown below is an example of the GAM results for the MDA8 at 616 regulatory stations for May-Sept 2018-2023:

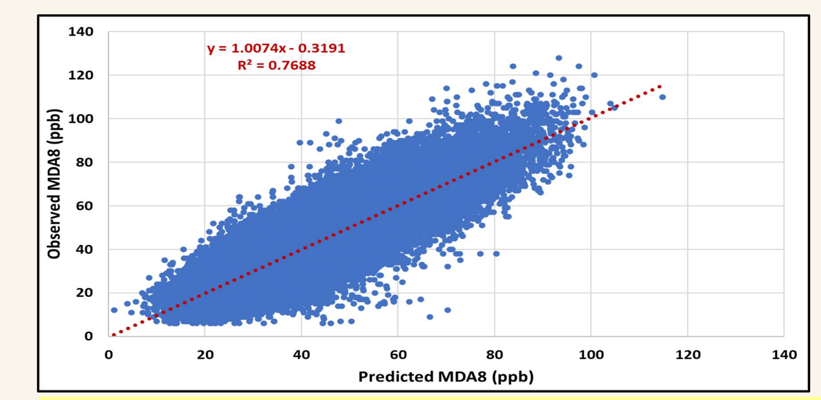

Figure 5. GAM/ML predictions of surface O_3 (MDA8) for 606 air quality sites. (Lee and Jaffe 2024)

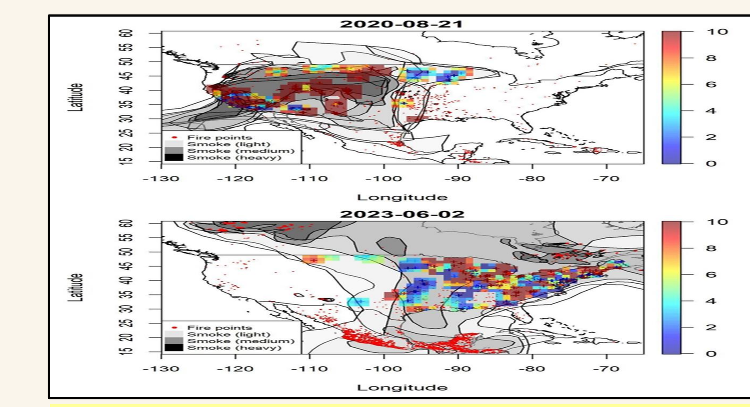

Figure 6. GAM estimated contribution to the MDA8 on two smokey days. (Lee and Jaffe 2024)

Because we can estimate the smoke contribution to the MDA8, this project is particularly relevant to states that may need to do exceptional event requests. However, the utility of the method depends greatly on the precision of the ML methodology. Satellite NO_2 and CH_2O will likely significantly improve these predictions and make the results more useful to state agencies and other decision makers.

Key questions for using these satellite data

Both projects will open new frontiers on what we can do with these satellite data. To be successful, we will have to address these questions:

1. How will noise in the NO_2 and CH_2O retrievals impact these results?
2. How much temporal averaging is necessary to get useful information from the TEMPO dataset?
3. For the GAM calculations of surface O_3, what time of day for the TEMPO observations provides the most useful information to forecast the daily MDA8 O_3?
4. Can we use the daily the NO_2 and CH_2O in a GAM framework to improve our O_3 predictions?
5. For smoky scenes, how accurate are the satellite retrievals for the NO_2 and CH_2O and how can we improve, correct and/or use these data in moderate to heavy smoke plumes?

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