**Assessment of Statistical Model Ozone Predictive Capability**

ABSTRACT

INTRODUCTION

Statistical regression-based models such as a multivariate linear regression models (Hubbard and Cobourn, 1998) and Generalized Additive Models (GAM) have been used extensive to predict O3 production using a variety of predictive factors which typically involve meteorology (Davis and Speckman, 1999; Ma et al., 2020; Thompson et al., 2001; Zheng et al., 2007). These types of models have been extended estimate the contribution of specific events (e.g., wildfire or stratospheric intrusion) to downwind O3 (Gong et al., 2017; Lee and Jaffe, 2024a; McClure and Jaffe, 2018).

The quantitative source attribution of daily predicted O3 in these types of methods typically involves a comparison of statistical model predicted daily O3 with observed levels on days considered impacted by a particular source and those not impacted by that source category (Gong et al., 2017; Lee and Jaffe, 2024a, b; Liu et al., 2018). This approach to source attribution assumes the underlying statistical model is accurately representing the contribution of weather and other sources and the only a single source is missing in its entirety.

A key question when considering model uncertainty is whether the model predicts O3 both higher and lower than monitored values at high concentrations (above 65 or 70 ppb) or whether the model displays systematic bias on these high monitored days. Statistical sampling presents additional challenges since high O3 days that are most policy relevant are few compared to the total number of measured monitor values and therefore not normally distributed around the mean of the model and the residuals are not representative of a normally distributed sample. In most cases, much of the positive residual can be attributed to the statistical variability of the regression model or other physical reasons for high O3 that are not related to specific sources. Typically, only some part of the concentration that is outside the normal range of variability (at the 95th percentile) could potentially be from a specific source, not the full residual.

It is critically important that inferences made based on statistical models be corroborated with meteorological patterns and more complex tools showing impacts (e.g., photochemical models or Lagrangian dispersion models). All these pieces of information should be consistent showing that high O3 impacts were the result of transport of smoke from fire rather than being dominated conducive meteorology coupled with sources for that area. For instance, in some situations the residual predicted by the GAM may be related to inadequate representation of regional stagnation events or inability to capture very localized features known to contribute to local O3 formation (e.g., complex land-water interface).

Certain weather conditions are needed to favor warm season O3 formation locally and regionally. These conditions include locally warm temperatures, clear skies, and light (or stagnant) winds (Sillman and Samson, 1995). Meteorology favoring regional transport of ozone and precursors from emissions sources outside the local area can also contribute to high ozone concentrations (National Research Council, 1992). These same weather conditions can lead to increases in anthropogenic and biogenic emissions of NOX and VOC which are both needed to initiate and enhance photochemical production of O3 (Sillman and Samson, 1995). These types of weather conditions are common in the central and eastern U.S. during the late spring and summer which often coincides with wildfire season making it challenging to discern whether high O3 was the result of these weather conditions or more distant sources like wildfires.

Higher than usual temperatures can lead to increased demand for air conditioning. This increased demand on energy systems would result in higher emissions of NOX, which is an important O3 precursor as much of the central and eastern U.S. have O3 formation chemistry that most frequently needs NOX to produce O3 (NOX limited areas) (Koplitz et al., 2021). Microbial activity in soil can result in NO emissions and these processes are temperature dependent meaning emissions are higher when temperatures are higher (Romer et al., 2018). Biogenic VOC emissions are typically abundant in the summer after leaf-out and strongly dependent on solar radiation and temperature (Guenther et al., 1993; Kesselmeier and Staudt, 1999). Higher levels of local to regional scale VOC available for O3 production reactions (Chameides et al., 1988).

The stratosphere can be a source of O3 in North America and tends to be highest during the cooler seasons. Stratospheric O3 most often reaches the surface in areas with high terrain like the western U.S. but can persist and be transported into other areas especially in the late spring (less photochemical activity) and areas with less sources of NOX emissions (central U.S.) which allows for a longer residence time in the atmosphere (Jaffe et al., 2018).

In North America, the fire season generally starts in spring and extends into fall with the specific timing varying widely by region. Fires also exhibit significant year to year variability, with emissions varying by an order of magnitude between high and low fire years in some places (Van Der Werf et al., 2017). Fires can contribute both to regional background and episodic surface pollution enhancements (Jaffe et al., 2018; McClure and Jaffe, 2018). Wildland fires emit particles and gas phase precursors that can react in the atmosphere to form ozone (O3) and other pollutants (Brey and Fischer, 2016; Hu et al., 2008; Langford et al., 2023; McClure and Jaffe, 2018; Rickly et al., 2023; Urbanski, 2014). Wildland fire smoke impacts on ozone (O3) are complex and likely dependent on many competing factors in the plume’s physical and chemical environment, both near the fire and as these factors change as the plume moves downwind. Variation in fuels, size, combustion efficiency, radiative impacts, and non-linear chemical interactions make estimating emissions and pollutant concentrations downwind of fires challenging (Jiang et al., 2012).

Recent research suggests O3 from wildfire that impacts areas far downwind is largely O3 formed very near the location of the fire and VOC that transports downwind (Jin et al., 2023; Rickly et al., 2023). Since areas where O3 production that is limited by VOC are small in size and these conditions are infrequent over time (Koplitz et al., 2021) fires and stratospheric natural sources can be notable contributors to well-mixed background O3 in North America and episodically may also contribute to distinct plumes of elevated background O3.

HMS smoke polygons represent potential smoke over a particular area but do not have any information about whether the smoke was at the surface, lofted, or both. Since these HMS smoke polygon products often provide no information about surface level impacts (Liu et al., 2023) additional analytics are needed to understand surface level air pollution from wildfire. \*\*new Owen Cooper paper shows disconnects between surface PM2.5, O3,and HMS smoke polygons; could reference that here\*\*

Forward and backward (HYSPLIT) trajectory tools were used to provide more information about source-receptor relationships to corroboration other analytics presented here. HYSPLIT is a trajectory model that uses 3D meteorology analysis fields to calculate forward and backward air mass trajectories (Stein et al., 2015). Chemical transport models use 3D meteorology to move air parcels forward in time through 3-dimensional space and account for chemical and physical (wet and dry deposition) processes in the atmosphere that impact residence time. Chemical transport models can be advantageous for tracking smoke from fire because many thousands of fires can be tracked simultaneously from different origins and when configured they can be differentiated by political boundary.

METHODS

RESULTS AND DISCUSSION

IMPLICATIONS

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