Wildland Fire Activity and Modeled Impacts on O3 and PM2.5

EPA-454/R-22-002
March 2022

Wildland Fire Activty and Modeled Impacts on O3 and PM2.5

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Air Quality Assessment Division
Research Triangle Park, NC

BACKGROUND

In the northern hemisphere, 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). Smoke from fires affects most of the contiguous U.S. at some point during the year. Fires across western states and parts of Canada can contribute both to regional background and episodic surface pollution (e.g., $PM_{2.5}$, O_3) enhancements (McClure and Jaffe, 2018).

Wildland fires emit particles and gas phase precursors that can react in the atmosphere to form ozone and other pollutants (Hu et al., 2008; Prichard et al., 2019; Urbanski, 2014). Understanding the air quality degradation from wildland fires is therefore a priority for air quality managers. Quantifying emissions of specific pollutants from wildland fires is a challenging task for many reasons, including uncertainties in underlying activity data, fuel characterization, and emission factors. Implementing fire emission inventories into photochemical models offers an opportunity to estimate air quality impacts from fires at local, regional and national scales.

Wildland fire smoke impacts on ozone (O_3) 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).

This document is intended to provide an overview of wildland fire activity, emissions, and downwind air quality (O_3 and $PM_{2.5}$) impacts. Fire activity and an emissions-based screening approach are provided annually for multiple years to illustrate year to year variability in fire activity and size. Photochemical grid modeling for 2018 provides O_3 and $PM_{2.5}$ impacts differentiated by fire type (e.g., wild, prescribed, and agricultural) and time of year to provide information about the location and timing of fire activity within a particular year. Hypothetical fires are used to explore potential local to continental scale impacts of various sized fires in different parts of the United States on downwind O_3 and $PM_{2.5}$ formation. This information is collectively intended to present information about when and where fire activity is common and how far downwind impacts on O_3 and $PM_{2.5}$ concentrations could be expected for fires located in different parts of the country. Finally, information is provided about where to find sources of information to support fire impact assessments on O_3 and $PM_{2.5}$ with some discussion about the strengths and weaknesses of different types of data for situations where the fire and downwind monitor are fairly close (tens to hundreds of miles apart) or very distant (hundreds to thousands of miles apart).

WILDLAND FIRE ACTIVITY

Fire detections are made from geostationary and polar orbiting satellites using both shortwave infrared and visible imagery products made available from the Hazard Mapping System (HMS) (Brey and Fischer,

2016; Hu et al., 2016). Fire detections are included in this analysis from multiple satellites reporting data. Fire detections may be missed by satellites when masked by clouds (Loría-Salazar et al., 2016) or when the size of the fires are below detection capability (Hu et al., 2016). Fires with short duration outside the overpass window of polar orbiting satellites may also be undetected and not reported.

Figure 1. Number of HMS fire detections aggregated for the entire year.

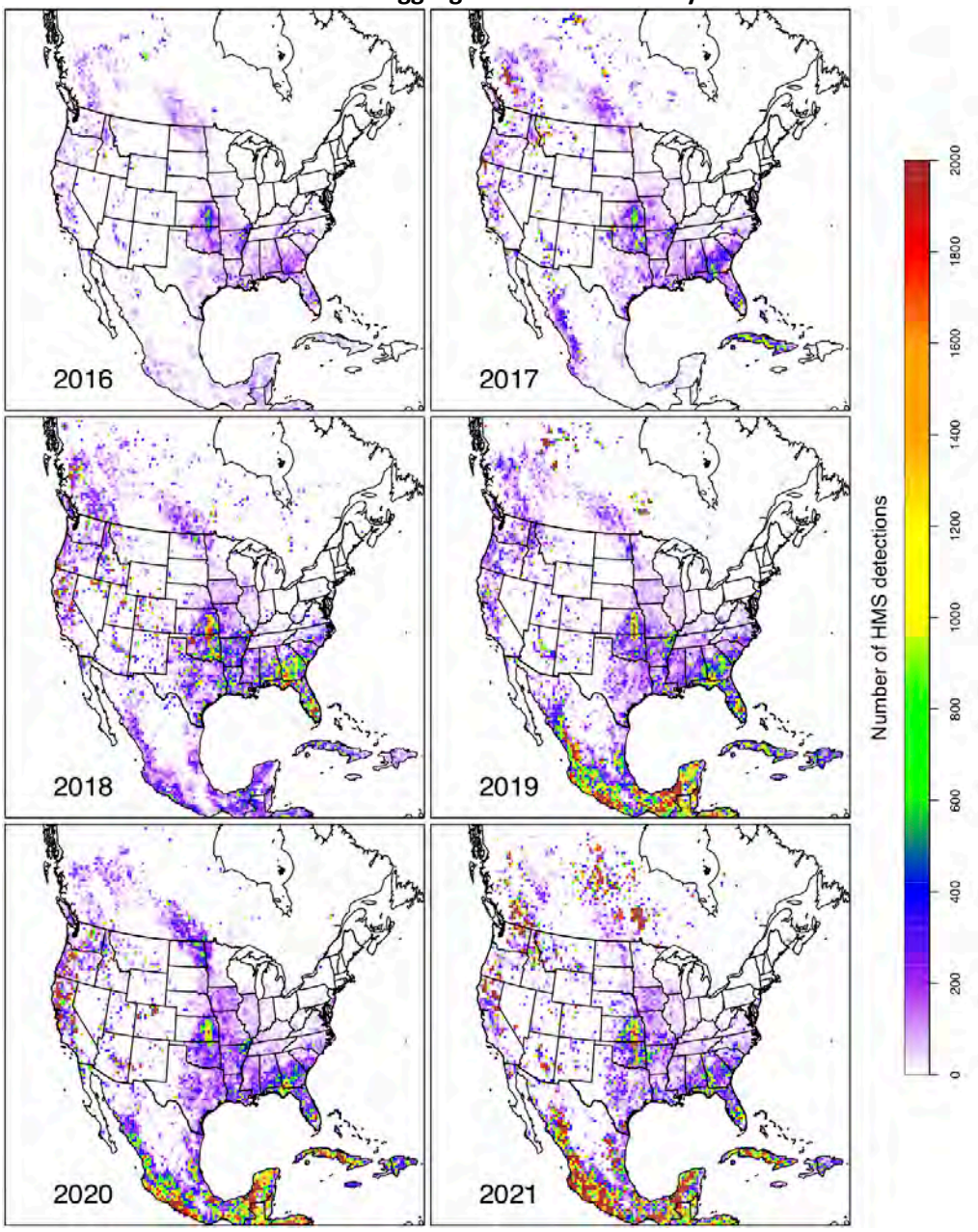


Figure 1 shows HMS fire detections aggregated over an entire year. Widespread fire activity is evident for each year in the southeast and midwest due to numerous prescribed fires in those areas. The number of fire detections provides an indication about frequency of fire activity in a particular area but does not directly translate to emissions strength or level of impacts on air quality.

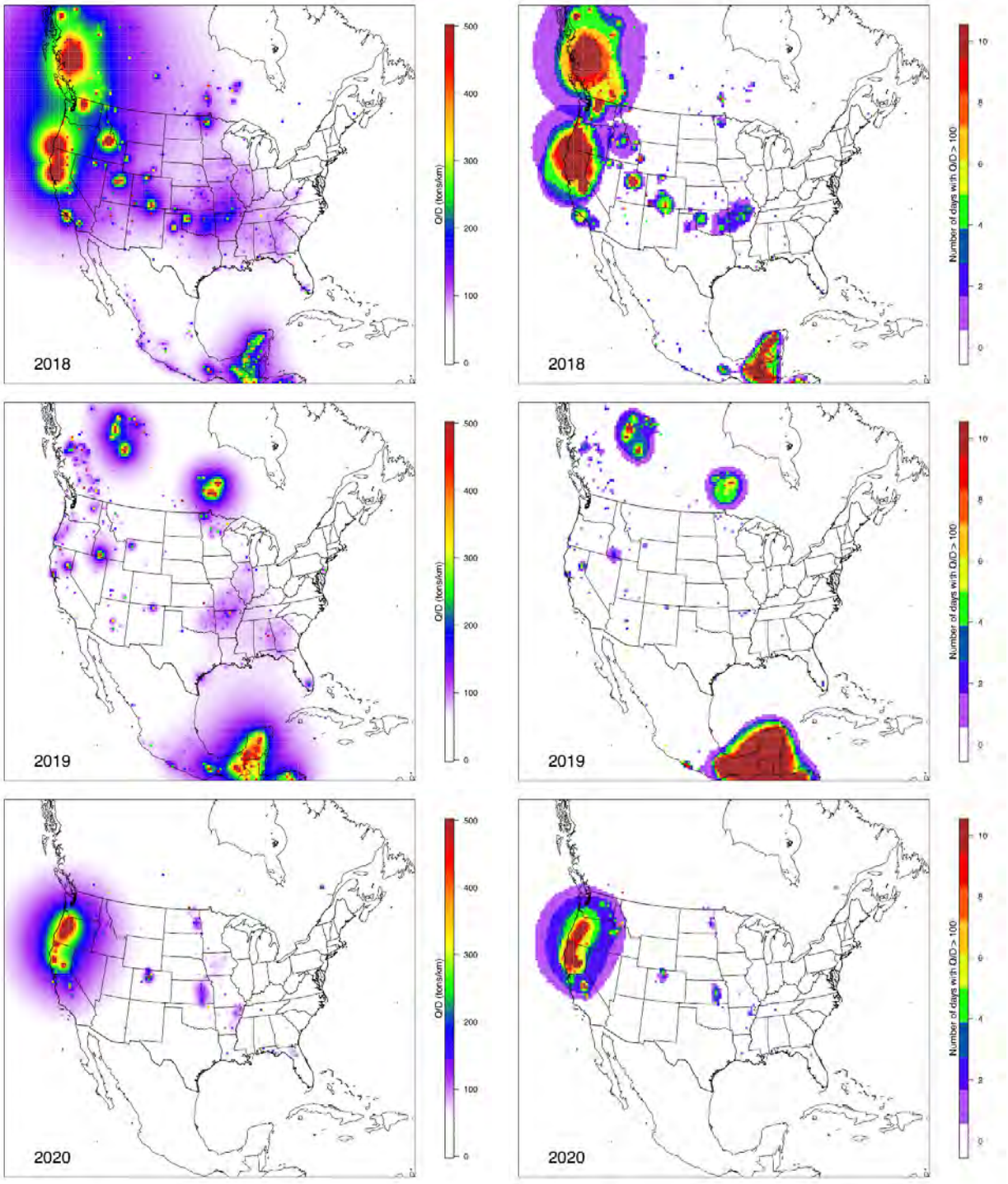
SCREENING APPROACH: EMISSIONS & DISTANCE (Q/D)

Wildland fire emissions provide a better estimate of where fire size and potential air quality impacts were highest than activity data (HMS fire detections) alone. One way to provide wildland fire emissions in the context of potential O_3 impacts is to sum nitrogen oxides (NO_X) and reactive VOC emissions (Q) for each fire and divide by distance (D) between the fire and location of interest (U.S. Environmental Protection Agency, 2016). Q/D was calculated using wildland fire emissions input files for the Community Multiscale Air Quality (CMAQ) modeling system. Wildland fire emissions input files for CMAQ have hourly emissions for each modeled species provided for specific days. Each day of the year has a different CMAQ input file for wildland fire emissions. Daily total emissions of NO, NO_2, and reactive VOC species were summed for each emissions release point on the wildland fire CMAQ input file. A set of gridded receptors was developed that matches a 12 km contiguous U.S. domain.

The distance from each wildland fire was then calculated to each gridded receptor. This process was repeated for each fire on each day specific emissions input file. The Q/D for each fire in each grid cell was kept and then summed over all fires for that day to derive a daily Q/D at each receptor location from all fires for that day. The CMAQ input files do not have names associated with each of the wildland fire emissions release points so tracking fire specific emissions with this process is not possible. However, this approach does provide a conservative estimate of wildland fire impacts since all fires over all days were aggregated.

Figure 2 shows emissions by distance for all wildland fires for 2018, 2019, and 2020. Daily Q/D impacts have been aggregated over the entire year. Figure 2 also shows a count of the number of days with Q/D exceeding 100. This is a very conservative estimate of Q/D and only intended to illustrate areas that may have experienced large wildland fire impacts during the year. For policy purposes, exceptional events demonstrations require daily Q/D values, not annual aggregate information as provided in Figure 2. The annual total Q/D values show that wildland fire emissions were notable in western Canada and western United States during multiple years and these impacts often lasted multiple days to weeks.

Figure 2. Annual sum of daily total emissions of wildland fire NO_X and reactive VOC by distance (Q/D) (left panel) and a count of Q/D values that exceed 100 (right panel) for 2018 (top row), 2019 (middle row), and 2020 (bottom row).



PHOTOCHEMICAL MODELING

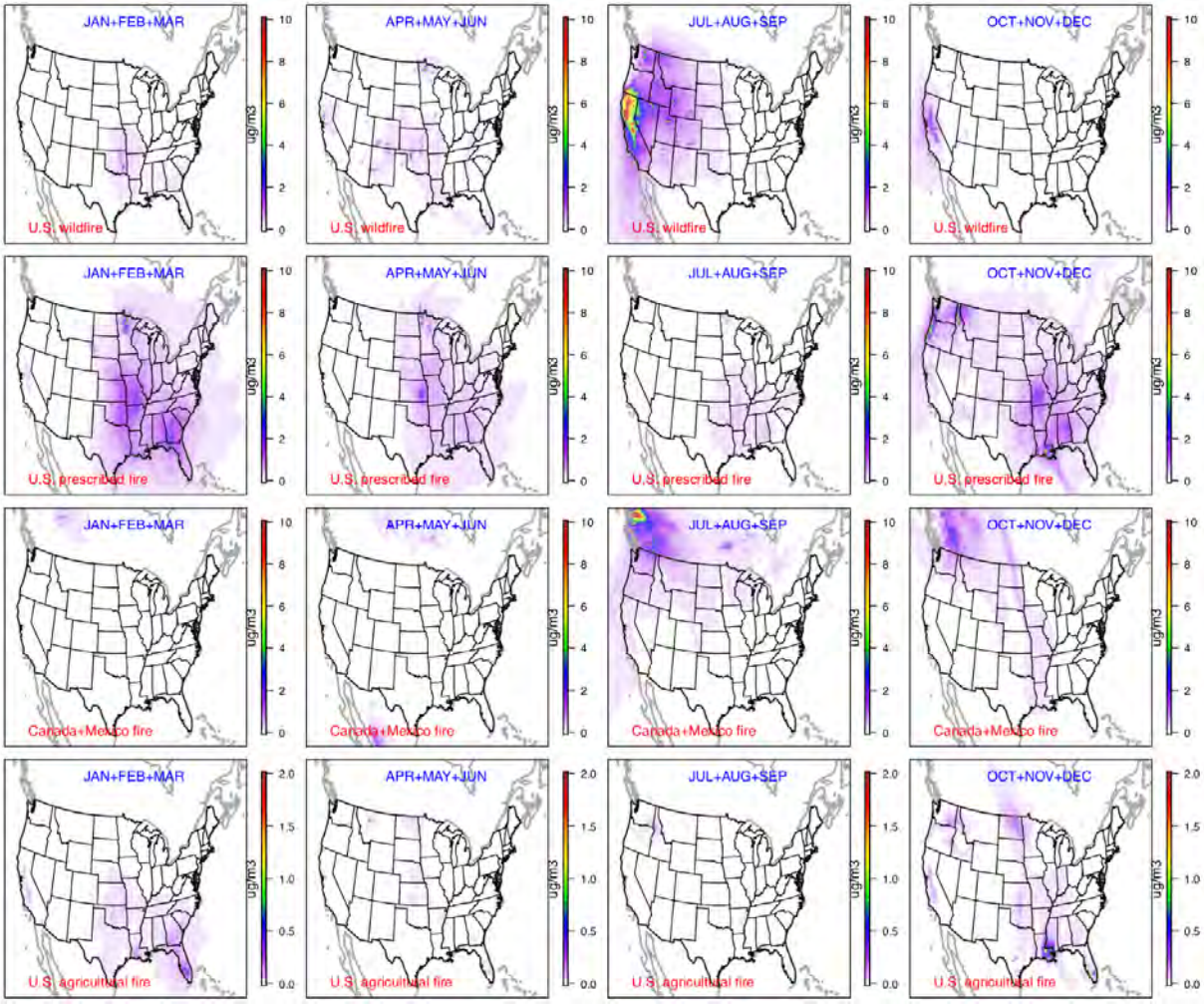
Photochemical modeling was done for the entire year of 2018 to illustrate fire impacts on O_3 and $PM_{2.5}$. The model was applied for a baseline configuration and multiple sensitivities to examine predicted $PM_{2.5}$ and O_3 impacts downwind. A series of hypothetical wildfires were modeled for periods of observed high O_3 from the summer of 2018 to illustrate how fire size (acres) impacts model predicted $PM_{2.5}$ and O_3 and how these impacts change over time and space. More details about the emissions and photochemical modeling are provided in Appendix A.

Previous studies using the Community Multiscale Air Quality (CMAQ) model to predict wildland fire impacts capture day to day variation in $PM_{2.5}$, although specific days may be notably over- or under-predicted (Baker et al., 2016; Kelly et al., 2019). Further, when activity data including fire size and timing are accurate, the model does well capturing plume placement vertically and downwind (Baker et al., 2018; Zhou et al., 2018). Model predictions of O_3 from wildfire tend to be systematically overpredicted at the surface (Baker et al., 2016; Baker et al., 2018). Predicting O_3 is challenging since O_3 production can be highly variable in space and time. For instance, at the fire O_3 production is largely inhibited by fresh nitric oxide (NO) emissions. Further downwind, O_3 may be produced at the top of the plume where precursors and sunlight are abundant, but not mix down to the surface.

PHOTOCHEMICAL MODEL ASSESSMENT: 2018 FIRE IMPACTS

Figure 3 shows 2018 quarterly averaged $PM_{2.5}$ impacts from multiple categories of fire: U.S. wildfire, U.S. prescribed fire, U.S. agricultural fire, and Canada and Mexico fires. It is important to note that the scales for the different types of fire are different so that spatial patterns of impacts can be discerned. The modeling shows that wildfire impacts were largest in 2018 during the traditional summer fire season. Prescribed fire impacts were highest during the non-growing season (winter). The impacts of agricultural burning were smaller than wild and prescribed fire but could be important in some locations during certain times of the year.

Figure 3. 2018 seasonal average $PM_{2.5}$ impacts from U.S. wildfire, U.S. prescribed fire, Canada and Mexico fire, and U.S. agriculture. Note that scales differ between categories to emphasize spatial patterns. FEPS emission factors were used for this assessment.



PHOTOCHEMICAL MODEL ASSESSMENT: HYPOTHETICAL FIRE IMPACTS

The photochemical model was applied with hypothetical wildfire in different parts of the United States to generate direct relationships between fire size (in terms of acres) and downwind $PM_{2.5}$ and O_3 impacts. Each hypothetical fire was modeled for more than one size (based on total acres) and for multiple episodes of high O_3. This was done to capture meteorological variability in potential O_3 formation in different parts of the country and focus the assessment on days more likely to have regulatory importance.

The hypothetical files were based on SERA emission factors, standard speciation profiles, and used the standard temporal profiles for wildfire. Multiple fire sizes were modeled based on daily acres burned: 50,000 and 100,000 acres. A total of 11 locations were selected to represent areas that historically have

wildfire activity or that could in the future (Figure 4). Each hypothetical fire was modeled for 13 different episodes representing multi-state high O_3 during 2018: June 6, 8, 18; July 2, 9, 10, 13, 14, 16, 29; August 2, 3, 4. Each of these episodes were a total of 5 days in length. The hypothetical fire was assumed to last for 24 hours (midnight to midnight local time) and was applied for the 2nd day of the 5-day period so that the downwind extent of impacts on subsequent days could be clearly discerned in the model output.

Figure 4. Location of hypothetical wildfires used in this assessment.

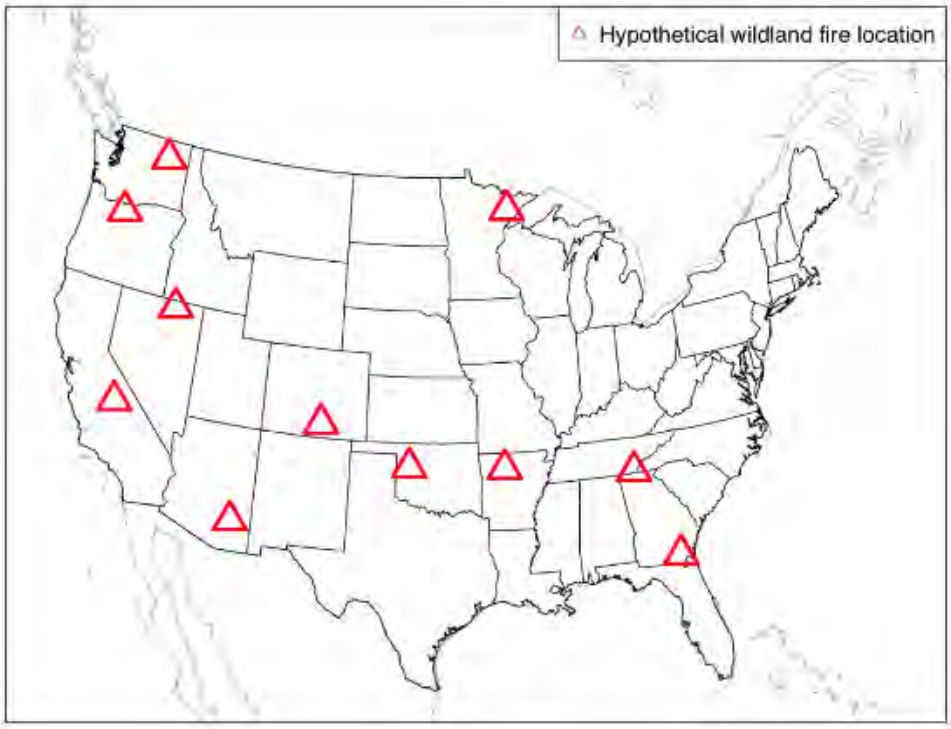


Figure 5 shows the distribution of emissions for multiple pollutants (NO_X, VOC, primary $PM_{2.5}$, and CO) for each of the fire locations for 4 different sized fires (50000 and 100000 acres) per location. Only the larger fire sizes were modeled with the photochemical model. This Figure shows the site-to-site variability in fuel loading and type that can result in comparatively smaller or larger emissions.

Figure 5. Emissions for each of the fire sizes at each of the locations as shown in Figure 7.

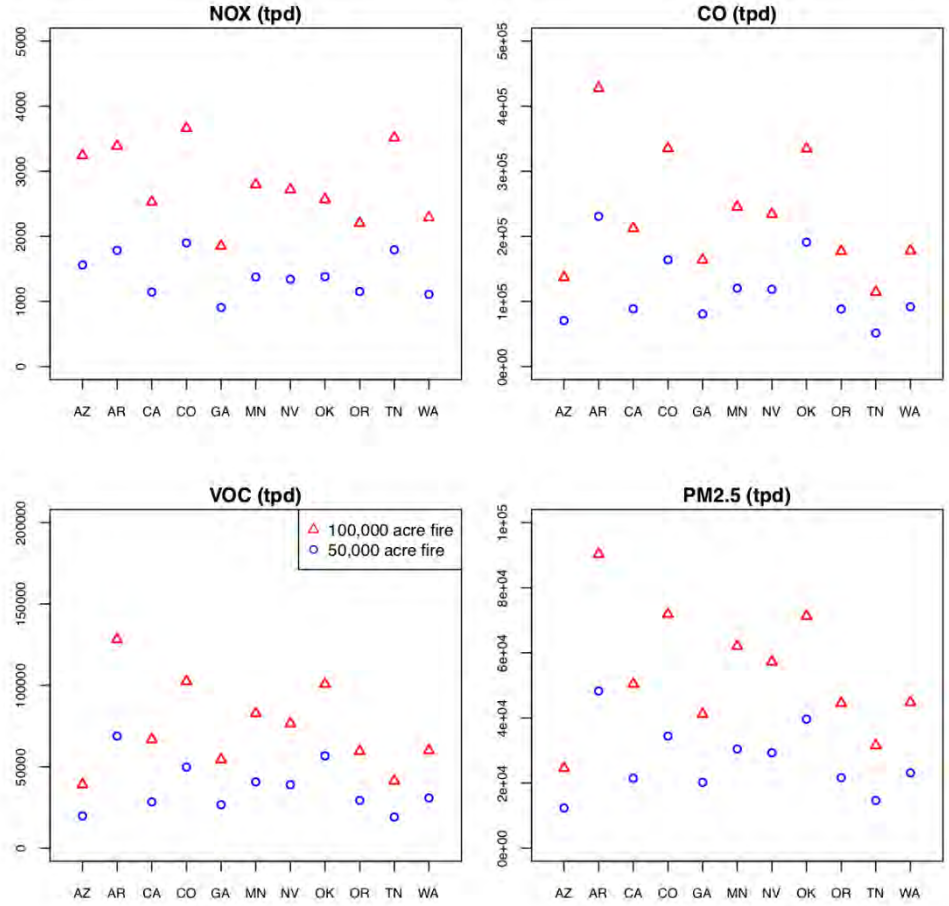


Figure 6 shows the modeled $PM_{2.5}$ and O_3 impacts of a hypothetical 50,000 acre fire in southern Arizona for one of the 13 episodes. The plume is closest to the location of the hypothetical fire on the first day the fire was modeled and transports downwind to the north and east due to prevailing winds moving in that direction. The $PM_{2.5}$ concentrations due to this hypothetical fire become smaller and more dispersed as the plume moves downwind from the initial release location. It is also evident in Figure 6 that the highest $PM_{2.5}$ impacts do not necessarily coincide with high O_3 impacts in space and time downwind. However, areas with the highest O_3 impacts do typically show some enhancement of $PM_{2.5}$.

Figure 6. Modeled $PM_{2.5}$ (top row) and MDA8 O_3 (bottom row) impacts from a hypothetical 50,000 acre fire in southern Arizona for a single 5 day episode.

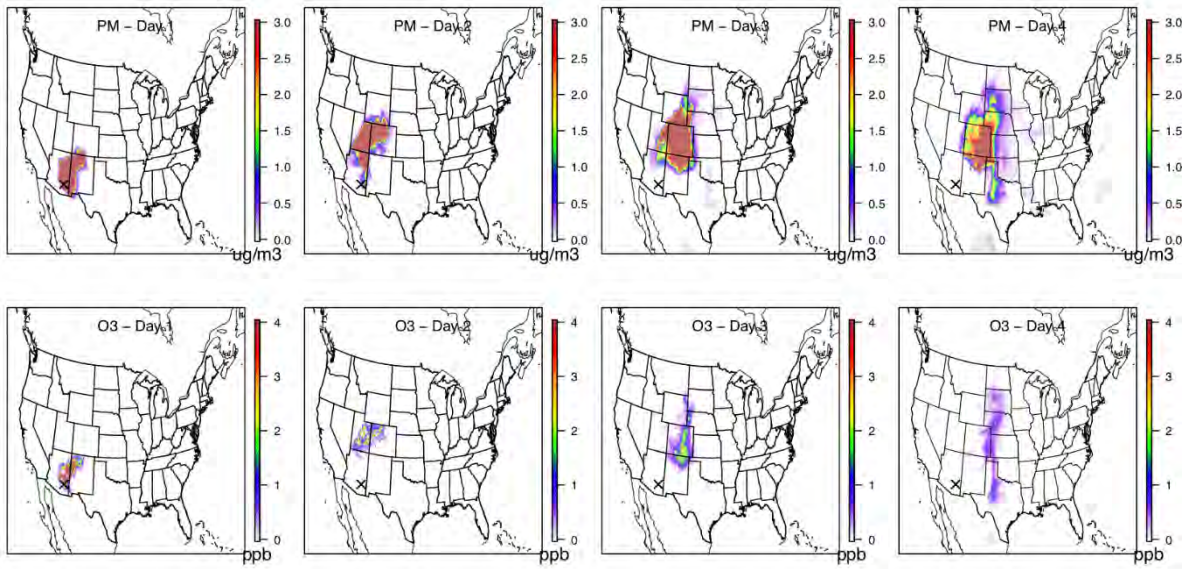


Figure 7. Downwind modeled impacts from a hypothetical 50,000 acre fire in southern Arizona: aerosol optical depth (top left), O_3 (top right), $PM_{2.5}$ (bottom left), and CO (bottom right). Impacts shown for 10 pm UTC July 4, 2018.

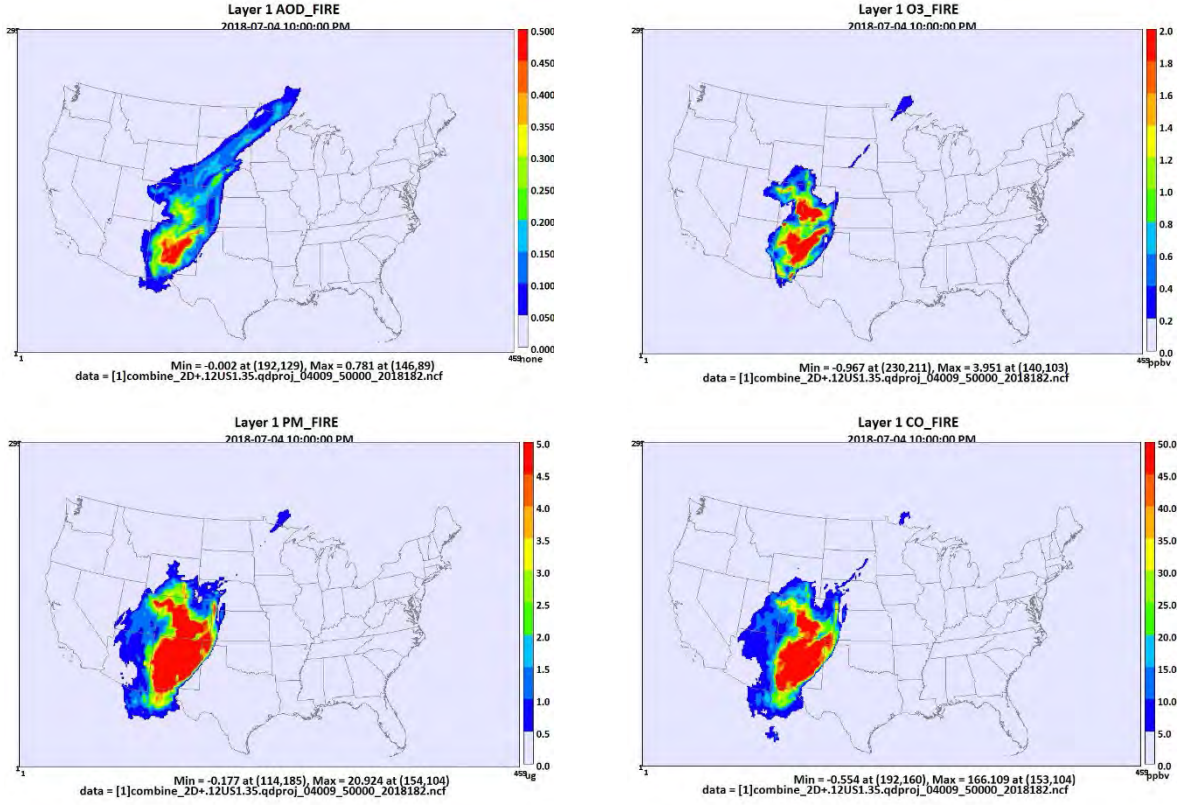


Figure 7 shows downwind impacts from a hypothetical 50,000 acre fire in southern Arizona for a particular hour. A similar downwind areal extent of impacts is modeled for PM2.5 and carbon monoxide, both largely primarily emitted and minimally impacted by atmospheric chemistry on the time scale of these multi-day modeling episodes. The footprint of O3 impacts is not quite as large as PM2.5 and carbon monoxide. The aerosol optical depth shows a larger downwind impact. Aerosol optical depth represents the entire column which indicates that the smoke has become lofted and decoupled from the surface when compared to the surface level impacts of the other pollutants shown in Figure 7. This shows that AOD is most consistent with surface level PM2.5 and O3 impacts closer to the fire (hundreds of miles away but not thousands).

Modeled $PM_{2.5}$ (Figure 8) and MDA8 O_3 (Figure 9) impacts are summarized for all hypothetical wildfires included in this assessment by distance from the fire, location, days of transport from the fire, and fire size. Even though the hypothetical fires modeled are the same in terms of the number of acres, the downwind impacts vary by location. This is because each location has different types of fuel and amounts of fuel which impacts the amount of emissions released in the atmosphere (see Figure 5). Another factor leading to regional variation in air quality impacts includes complex terrain, proximity to large water bodies (with shallow mixing layers leading to high surface levels of pollution), and weather which can impact mixing layer heights and temperatures for photochemistry among other factors.

The distribution of $PM_{2.5}$ and MDA8 O_3 impacts were higher for the larger fire size. Even though the larger fire size (100,000 acres) was double the smaller size fire (50,000 acres) the downwind impacts were often less than twice as large as the smaller fire.

Both $PM_{2.5}$ and MDA8 O_3 impacts are highest at distances very near the fire location (less than 100 km) and decrease as distance from the fire increases. Impacts for both also decrease as days of transport downwind increase. However, this is much more pronounced for O_3 than $PM_{2.5}$ as the distribution for $PM_{2.5}$ impacts is fairly similar for the first and second day while O_3 impacts notably decrease for each day of transport downwind. The majority of the MDA8 O_3 impacts (shown as the interquartile range in Figure 8) from all of the hypothetical sources modeled over all of the different episodes and fire sizes (50,000 and 100,000 acres) are very small compared to the level of the 8-hr O_3 National Ambient Air Quality Standard at distances greater than 1000 km. The maximum MDA8 O_3 impacts at these distances downwind from wildfire (greater than 1000 km) are below the average U.S. anthropogenic emission contribution to MDA8 O_3 and well below the U.S. anthropogenic emission contribution to most urban areas in the central and eastern United States (U. S. Environmental Protection Agency, 2020).

Figure 8. The distribution of daily average $PM_{2.5}$ impacts from all hypothetical sources modeled as part of this assessment.

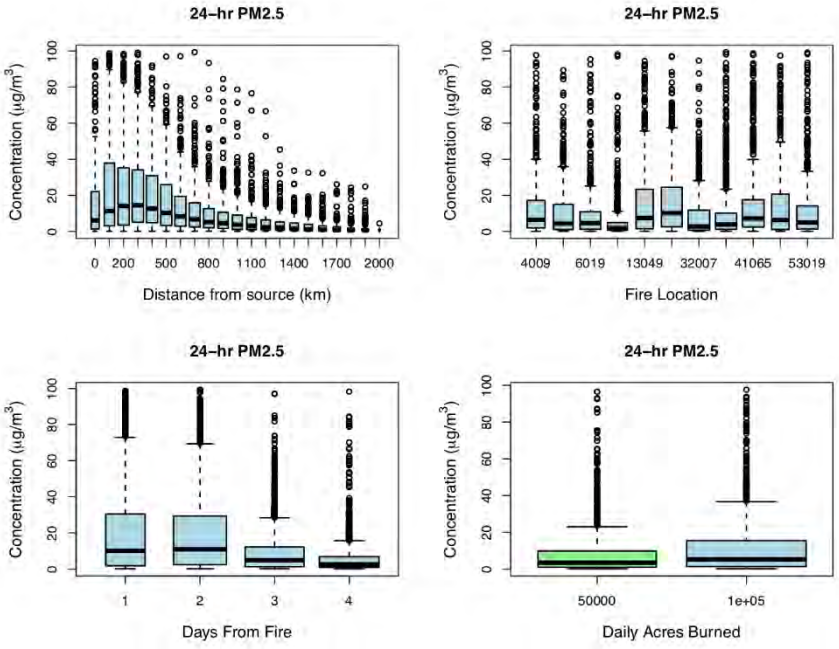


Figure 9. The distribution of MDA8 O_3 impacts from all hypothetical sources modeled as part of this assessment.

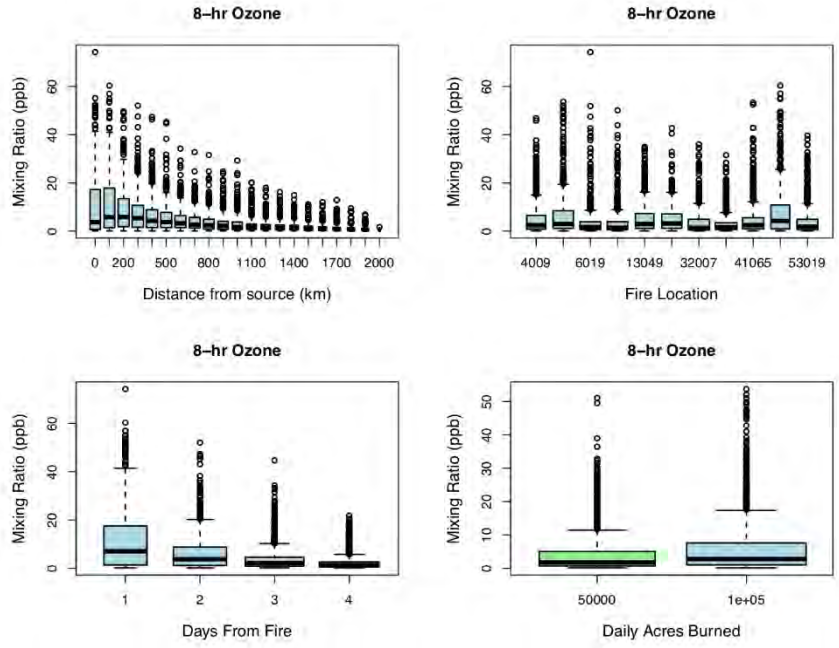


Table 1 shows model predicted MDA 8 O_3 and daily average $PM_{2.5}$ impacts from all hypothetical fires modeled as part of this assessment for multiple percentiles. The impact is shown for the day of the fire (day 1) and subsequent days transported downwind. This information is provided for the 50,000 and 100,000 acre fires (over a single day), which are large fires. The values in this table are not intended to provide information about downwind impacts at specific monitors. This table is intended to provide very conservative estimates of downwind impacts from large fires to provide context about potential source-receptor impacts. The impacts shown in Table 1 do not exclude modeled days with low levels of O_3 or $PM_{2.5}$ which means some of these impacts could be on days with low levels of pollution.

Table 1. 98th percentile model predicted impacts from all hypothetical wildfire included in this assessment. Day 1 is the day the 50,000 or 100,000 fire burned in the model and subsequent days represent downwind transport (and no additional acres burned).

		Daily $PM_{2.5}$ Concentration (µg/m^3)			
Acres	Percentile	Day 1	Day 2	Day 3	Day 4
100,000	0.98	88	83	46	26
50,000	0.98	87	65	28	15
100,000	0.95	77	69	33	18
50,000	0.95	72	48	19	10
100,000	0.90	62	51	24	13
50,000	0.90	51	35	14	7
100,000	0.75	30	29	12	7
50,000	0.75	25	18	7	4

		MDA8 O_3 Mixing Ratio (ppb)			
Acres	Percentile	Day 1	Day 2	Day 3	Day 4
100,000	0.98	47	25	17	11
50,000	0.98	40	18	11	6
100,000	0.95	36	18	11	7
50,000	0.95	30	14	7	4
100,000	0.90	29	14	8	5
50,000	0.90	24	10	6	3
100,000	0.75	17	9	5	3
50,000	0.75	15	6	3	2

ANALYTICS FOR SPECIFIC FIRE IMPACT ASSESSMENTS

A variety of analytics could be useful for characterizing the impacts of specific fire events on O_3 and PM concentrations. This section is intended to provide information about where to obtain information for developing a conceptual description of a fire impacting a specific monitor and provide an overview of analytics that might be useful for supporting a causal relationship between smoke from a particular fire

and a downwind monitor. Some explanation is also provided in the following sections about why some analytics might be considered useful for O_3 or PM demonstrations showing wildfire impacts on near or far downwind surface level monitors. Some products may be more useful for situations where the fire and potentially impacted monitor(s) are nearby and might not be worth including for demonstrations where the transport distances are much greater. Further, some products may be more useful for either PM or O_3 impact assessments rather than being equally useful for both.

While individual tools and datasets have limitations, using multiple sources of corroborative evidence to support an exceptional event demonstrate can result in a stronger case. Further, more evidence and the use of more sophisticated tools are needed in situations where monitors are far downwind (e.g., hundreds to thousands of miles downwind) of a fire. A single analysis is not sufficiently demonstrative of an exceptional event impact on its own, even for the simplest cases. A demonstration should integrate information from several different analyses to sufficiently demonstrate the clear causal relationship between a fire and a monitored exceedance or violation.

Additional guidance and details on the types of analyses for this purpose can be found in the exceptional events Wildfire Ozone Guidance and the Updated Frequently Asked Questions documents (U.S. Environmental Protection Agency, 2016). For both O_3 and PM, EPA recommends that air agencies, in consultation with their EPA Regional office, use a simple to-complex stepwise approach for integrating only those analyses that are appropriate and necessary to satisfy the "clear causal relationship" criterion. This approach is intended to help conserve air agency resources and support the goal of right-sized demonstrations (U.S. Environmental Protection Agency, 2016). The analytics presented here are not organized in a manner consistent with the tiering system in the wildfire exceptional events guidance. Agencies intending to develop such demonstrations should follow that guidance and discuss with their EPA Regional office when determining what evidence is required for a particular demonstration.

Table 2. Sources of information that could support the development of the conceptual description of O_3/PM formation in an area and a particular fire impact episode.

Type	Location
Archived historical weather maps (surface and aloft continental scale)	https://www.spc.noaa.gov/obswx/maps/
Archived historical surface wind maps (local to regional scale)	https://www.airnowtech.org
Fire location	https://inciweb.nwcg.gov https://www.airnowtech.org https://worldview.earthdata.nasa.gov https://www.ospo.noaa.gov/Products/land/hms.html#data
Fire size (acres burned)	https://inciweb.nwcg.gov https://fsapps.nwcg.gov/ravg/data-access
Fire emissions	tools.airfire.org/playground/v3/emissionsinputs.php

Conceptual descriptions showing O_3 and PM impacts from specific fires include a description of synoptic scale meteorology linking the fire location and impacted monitor, fire size (and emissions if known), and an understanding about typical (non-fire related) meteorological conditions leading to elevated O_3 or PM in a particular area. Table 2 provides sources of information for the technical elements related to developing the conceptual model of the event and typical O_3/PM formation in an area.

Relating fire emissions to downwind surface level O_3 or PM impacts often requires more complicated analytics, especially in situations where the fire and monitor are far (e.g., hundreds to thousands of kilometers) apart. Table 3 provides simple analytic technical elements and Table 4 provides more complex approaches for supporting a causal relationship assessment. This section also includes some discussion about the strengths and weaknesses of these different analytics for O_3/PM impact assessments in situations where the fire and monitor(s) are closer in proximity (hundreds of miles apart or less) or more distant (hundreds to thousands of miles apart).

Table 3. Simple analytics supporting fire emissions affected the monitor(s).

Type	Location
HMS smoke polygons	https://www.airnowtech.org https://www.ospo.noaa.gov/Products/land/hms.html#data
Visible satellite images	https://worldview.earthdata.nasa.gov
AOD satellite product	https://worldview.earthdata.nasa.gov
NO_2, CO satellite products	epa.gov/hesc/remote-sensing-information-gateway
O_3/PM monitored spatial/diurnal patterns	https://www.epa.gov/aqs

HMS SMOKE POLYGONS

HMS smoke products are contours which represent human drawn lines based on satellite visible imagery (https://www.ospo.noaa.gov/Products/land/hms.html#about). Polygons are colored with a human interpreted correspondence to aerosol concentration somewhere in the vertical column but do not provide quantitative information of surface level O_3 or PM impacts. Documentation for this product specifically emphasizes the "qualitative nature of the visual analysis" when interpreting the smoke layers. These smoke sketches do not provide any information about whether smoke is at the surface or aloft in the atmosphere. The lightest shaded contour color represents the potential for smoke with an interpreted concentration ranging from 0 to 10 µg/m^3 somewhere in the column, which means areas with this shading might represent very small or no actual smoke impact, particularly at the surface. This suggests this product is most useful for understanding smoke impacts closer to fires and confidence would be highest for using the warmest color contours, recognizing that even in this situation the product does not provide information about smoke at the surface.

HMS smoke sketches are typically shown as an aggregate of multiple contours from multiple satellites (GOES-EAST and GOES-WEST) for a given day. When these polygons are superimposed, they can provide the appearance of a large smoke impact even though the HMS smoke sketches represent up to 4-hour

increments in time. In many situations presenting the contours in this way may provide reasonable information; however, when attempting to establish a causal relationship it is important to determine whether potential smoke impacts happen at relevant times of the day or progress through time in a way that would suggest a continuous impact from a particular location. HMS smoke sketches can provide useful information when impacts are large and can be corroborated with other information like visible images or monitoring data and trajectory analysis. This type of information is most useful for areas near large wildfires and less useful for supporting a connection between specific fires and areas hundreds to thousands of miles downwind, where smoke impacts are very uncertain and most likely lofted well into the free troposphere.

SATELLITE PRODUCTS

Multiple types of remotely sensed data derived from satellite products can provide an indication about whether smoke may be in the atmosphere. These include visible images that show clouds and smoke, HMS smoke products, aerosol optical depth (AOD), NO_2, and CO from one or more satellite platforms. Most satellite-based products do not provide information about surface level smoke, and none provide information about surface level O_3 or PM impacts from smoke.

Wildfires are not the only source of NO_2, CO, and aerosol in the atmosphere, so interpretation of these products for the purposes of identifying causality from specific fires to specific monitors over large distances can be challenging. For instance, NO_2 column data can provide useful information about large emissions sources but does not provide a clear link between sources and receptors far apart (i.e, hundreds to thousands of miles). Space-based measurements of NO_2 column collected by the TROPOMI satellite are useful for showing whether anthropogenic emissions at the monitor(s) are similar or greater than other large cities in North America for recent time periods (2018 and later) (Goldberg et al., 2019). Products like TROPOMI NO_2 may be valuable for supporting a conceptual description of typical O_3 or PM formation in a particular region.

AOD is the sum of optical influence across all aerosol species, often dominated by the more reflective anthropogenic aerosols like sulfate. Isolating a smoke signal with AOD on individual days is very difficult, especially away from very large emissions sources like wildfire or a complex of wildfires.

Visible images from satellites can be even more difficult to discern source-receptor relationships, especially when long distances are between the source and monitor. Additionally, large cloud complexes between the fire event and monitor(s) downwind can further complicate using these images to connect smoke to downwind O_3 or PM impacts. Often long-range transport of smoke is lofted by synoptic weather and transported in the free atmosphere decoupled from the surface. This transport can often be seen in the visible satellite images but does not mean smoke is being mixed to the surface.

SURFACE LEVEL AMBIENT DATA ANALYTICS

Some ambient data measurements that are more helpful than NO_2, CO, or $PM_{2.5}$ for specifically identifying fire impacts. This includes speciated PM compounds (e.g., elemental carbon), levoglucosan and other biomass burning tracers, black carbon/aethalometer data (differences between wavelengths measured by an aethalometer can be used as a fingerprint of smoke), and pollutant ratios (e.g., PM2.5/PM10, PM2.5/CO) that are notably different for smoke compared to urban or clean airsheds (U.S. Environmental Protection Agency, 2016). These types of analytics are considered valuable for

evaluating smoke impacts in an area by potentially providing source-specific, quantitative data supporting smoke impacts at ground level. Spatial and temporal analyses of monitoring data can also be informative. It is useful to compare potentially smoke impacted data to typical concentrations at that site for different periods of time: hourly, day-of-week, and seasonally rather than simply looking at time series for "peaks" that may simply be representative of local emissions and boundary layer dynamics.

Timeseries and statistical analysis could be used to show anomalies for multiple pollutants measured at a receptor(s) based on routinely measured data collected by state and local agencies. Coincident anomalous CO, $PM_{2.5}$, and O_3 concentrations could occur on some days with potential smoke impacts (Laing et al., 2017). It is most likely that fire impacted days might have coincidentally high $PM_{2.5}$, CO, and O_3 especially at monitors close to wildfires (Laing et al., 2017). However, these species being simultaneous elevated is also expected during stagnation events that are unrelated to fires. This relationship would likely be stronger for monitors in close proximity to wildfire rather than over a thousand miles apart. Showing these pollutants are coincidentally elevated on the same day is not evidence on its own to support a fire impact. Elevated NO_2 levels are likely more indicative of local emissions and meteorological conditions such as stagnation events than it is of fire impacts and is a poor tracer of fire activity.

Table 4. Complex analytics supporting fire emission transport to the monitor(s)

Type	Location
Trajectory analysis	ready.noaa.gov/HYSPLIT_traj.php
O_3 forecast modeling systems with wildfire emissions	None at the time of the development of this document
PM forecast modeling systems with wildfire emissions	https://tools.airfire.org https://rapidrefresh.noaa.gov/hrrr https://www.nrlmry.navy.mil/aerosol
Photochemical modeling	https://www.epa.gov/sites/default/files/2020-10/documents/O_3-pm-rh-modeling_guidance-2018.pdf

TRAJECTORY ANALYSIS (HYSPLIT)

The HYSPLIT model is a Lagrangian trajectory model that can track pollutants through 3-dimensional space either forward or backward in time from a particular location (Draxler and Hess, 1997; Li et al., 2020). Forward trajectories developed using the HYSPLIT model starting at the fire event and backward trajectories starting at the monitor(s) location are very useful for showing air from the fire event transported to the monitor(s) on the day(s) targeted for a demonstration. The forward and backward trajectories should be reasonably consistent with each other and consistent with local (for fires and monitors in close proximity) and continental scale meteorology (for fires and monitors hundreds to thousands of miles apart).

Multiple types of trajectories are possible at the HYSPLIT internet site. Analyses with multiple trajectories should provide a consistent pattern of transport from the fire to the site (rather than an individual trajectory or two out of a larger analysis). The trajectory frequency product is very useful for these types of assessments because these provide a sense about the likelihood of distant endpoints

traversing over a particular location and how often air was over a particular location. This type of information helps understand whether air on the days included in a demonstration tend to be more local in origin or from more distant areas.

The trajectory timing should be consistent with the conceptual model and the timing of the fire, the emissions, and the exceedances. For example, if a conceptual description indicates transport from a fire 2 days ago, the backward trajectory should be initiated from the monitoring site at a time consistent with the observed smoke and it should pass near the fire location around the time the fire was active.

The trajectories become more uncertain the further forward in time from a fire location and further backward in time from a monitor location. The trajectories also do not provide information about dry and wet deposition or chemical transformation of pollutants in an air parcel. For instance, a longer trajectory (e.g., greater than 2 days) would be more likely to have impacts from physical removal processes like deposition. Consideration of rain events between the source and receptor help understand the potential impact of wet deposition removing smoke from the atmosphere.

PHOTOCHEMICAL MODELS

Photochemical models can provide a useful connection between specific fires and downwind monitors (Baker et al., 2016; Baker et al., 2018; Hu et al., 2008; Liu et al., 2019). These models use meteorological inputs that are comparable and sometimes higher resolution than those used by HYSPLIT and would be expected to provide similar source-receptor information as HYSPLIT. A photochemical model can provide additional information that HYSPLIT cannot provide which is an estimate of O_3 and other chemicals from specific fires at specific monitors downwind when the model is configured and applied in a way to reasonably quantify these impacts. Photochemical grid models have been shown to overpredict O_3 from wildland fire (Baker et al., 2016; Baker et al., 2018), which means these models can provide an indication about whether specific fires impact certain downwind monitors, but the predicted levels may be overstated to a large degree.

PHOTOCHEMICAL MODEL FORECAST PRODUCTS

Some air quality forecast systems predict O_3 and $PM_{2.5}$ from wildland fire. Forecasting systems are not set up to provide information about specific fire impacts on specific downwind monitors. Forecasting systems predicting O_3 and $PM_{2.5}$ from wildland fire can also overstate impacts similar to retrospective photochemical modeling. Forecasting systems that do not include wildland fire emissions do not provide any information about the impacts from wildland fires on downwind monitors. The difference in forecasted O_3/$PM_{2.5}$ and observed O_3/$PM_{2.5}$ could be due to many reasons not related to the absence of wildland fires; poorly characterized stagnant meteorological conditions are challenging features for prognostic meteorological models. Factors such as day-specific emissions not being adequately captured (e.g., anthropogenic emissions) or other physical aspects of the modeling system such as representation of deposition and chemical reactions impact model performance. In 2020, the predictions of O_3 forecasting systems would particularly be challenged to represent high O_3 due to the extreme uncertainty in anthropogenic emissions resulting from area specific COVID impacts.

Several operational forecasts provide information about $PM_{2.5}$ impacts from wildland fire. The Naval Research Laboratory (NRL) has developed a global, multi-component aerosol analysis and modeling capability (NAAPS: Navy Aerosol Analysis and Prediction System) that combines satellite data streams

with other available data and the global aerosol simulation and prediction model for predicting the distribution of tropospheric aerosols.

NOAA's High Resolution Rapid Refresh-Smoke model (HRRR-Smoke) is a numerical weather prediction model that forecasts the impact smoke has on several weather variables. Based on satellite observations of fire location and intensity, HRRR-Smoke predicts the movement of smoke in three dimensions across the country over 48 hours, simulating how the weather will impact smoke movement and how smoke will affect visibility, temperature, and wind. Other smoke forecasting systems exist and could be used to support a demonstration (e.g., BlueSky system). A limitation with some forecast products for assessing links between specific fires and downwind monitors is that they may not provide surface level impacts of $PM_{2.5}$. Products that provide a total column integration means smoke could be anywhere in the atmosphere and as distance between a fire and monitor increases the impacts are more likely to be lofted in the upper troposphere.

Table 5 provides additional sources of information for multiple types of analytics that could be used to inform the technical components of a demonstration.

Table 5. Additional sources of information

Type	Location
Ceilometer data	alg.umbc.edu/ucn
O_3 lidar data	www-air.larc.nasa.gov/missions/TOLNet
Aerosol profiles (CALIPSO)	https://www-calipso.larc.nasa.gov/products/

GROUND-BASED LIDAR DATA

Ceilometers are ground-based instruments that make high time resolution measurements of the vertical profile of aerosol backscatter (Knepp et al., 2017; Liu et al., 2011). Ozone lidars are ground-based instruments that make high time resolution measurements of the vertical profile of ozone (Langford et al., 2019). Both typically measure through the extent of the troposphere although neither provide surface level information due to limitations with the technology (Chan et al., 2018; Langford et al., 2021). Both can provide valuable information about the vertical structure of the boundary layer on days that might be impacted by smoke. Certain types of vertical structure would tend to inhibit vertical mixing from upwind sources emphasizing local pollutant build-up and formation. These types of instruments can also be used with other sources of information to consider the potential for upper-level pollution to reach the surface impacting specific monitors. These instruments provide reasonable information about the vertical atmosphere near potentially impacted monitors (same urban scale airshed). Lidars placed hundreds or more miles away from important meteorological features impacting a certain monitor would not provide useful information for the impacts at that monitor. This means lidars that are hundreds of miles away from a potentially impacted monitor would not be useful for understanding that situation.

SATELLITE PRODUCTS (CALIPSO)

CALIPSO transects suffer limitations as uncertainty increases for near-surface data and the data is classified using source categorization that makes source attribution very difficult since many sources

could contribute similar types of pollution at the surface (Burton et al., 2013). CALIPSO products poorly distinguish between aerosol types, especially between urban (anthropogenic) and smoke (Burton et al., 2013). CALIPSO often categorizes aerosol as "smoke" where a higher resolution airborne HSRL instrument categorizes the same aerosol as "urban" in origin (Burton et al., 2013). Research indicates that CALIPSO is challenged when categorizing aerosol (Burton et al., 2013) and the "polluted dust" and "polluted continental/smoke" category should not by default be interpreted as smoke.

STATISTICAL REGRESSION MODELS

Statistical regression-based models such as a Generalized Additive Model (GAM) are sometimes used to relate the impacts from specific events (e.g., wildfire or stratospheric intrusion) with downwind 8-hour ozone exceedances. US EPA guidance (U.S. Environmental Protection Agency, 2016) states that "Users of regression models should consider the uncertainties in the model's prediction abilities, specifically at high concentrations, before making conclusions based on the modeled results. A key question when considering model uncertainty is whether the model predicts O_3 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." Further, 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 O_3 impacts were the result of transport of smoke from fire rather than being dominated by other more common 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 O_3 formation (e.g., complex land-water interface).

Statistical sampling presents additional challenges with these types of analytics since exceptional events demonstrations typically are focused on the highest measured monitor values and therefore are not normally distributed around the mean of the model and the residuals for those points 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 O_3 that are not related to specific fires. EPA guidance is clear that the "minimum fire contribution" is not the full residual, but rather the difference between the residual and the 95th confidence interval for the statistical model uncertainty (U.S. Environmental Protection Agency, 2016). The means that only some part of the concentration that is outside the normal range of variability (at the 95^{th} percentile) could potentially be from a specific source like a fire, not the full residual.

REFERENCES

Baker, K., Woody, M., Tonnesen, G., Hutzell, W., Pye, H., Beaver, M., Pouliot, G., Pierce, T., 2016. Contribution of regional-scale fire events to ozone and PM 2.5 air quality estimated by photochemical modeling approaches. Atmospheric Environment 140, 539-554.

Baker, K., Woody, M., Valin, L., Szykman, J., Yates, E., Iraci, L., Choi, H., Soja, A., Koplitz, S., Zhou, L., 2018. Photochemical model evaluation of 2013 California wild fire air quality impacts using surface, aircraft, and satellite data. Science of The Total Environment 637, 1137-1149.

Bash, J., Baker, K.R., Beaver, M., 2015. Evaluation of improved land use and canopy representation in BEIS v3. 61 with biogenic VOC measurements in California. Geoscientific Model Development Discussions 8, 8117-8154.

Brey, S.J., Fischer, E.V., 2016. Smoke in the city: how often and where does smoke impact summertime ozone in the United States? Environmental science & technology 50, 1288-1294.

Burton, S., Ferrare, R., Vaughan, M., Omar, A., Rogers, R., Hostetler, C., Hair, J., 2013. Aerosol classification from airborne HSRL and comparisons with the CALIPSO vertical feature mask. Atmospheric Measurement Techniques 6, 1397-1412.

Chan, K.L., Wiegner, M., Flentje, H., Mattis, I., Wagner, F., Gasteiger, J., Geiß, A., 2018. Evaluation of ECMWF-IFS (version 41R1) operational model forecasts of aerosol transport by using ceilometer network measurements. Geoscientific Model Development 11, 3807-3831.

Cubison, M., Ortega, A., Hayes, P., Farmer, D., Day, D., Lechner, M., Brune, W., Apel, E., Diskin, G., Fisher, J., 2011. Effects of aging on organic aerosol from open biomass burning smoke in aircraft and laboratory studies. Atmospheric Chemistry and Physics 11, 12049-12064.

Draxler, R.R., Hess, G., 1997. Description of the HYSPLIT4 modeling system.

Emery, C., Jung, J., Koo, B., Yarwood, G., 2015. Improvements to CAMx Snow Cover Treatments and Carbon Bond Chemical Mechanism for Winter Ozone. Prepared for the Utah Department of Environmental Quality, Division of Air Quality, Salt Lake City, UT. Available at: http://www.camx.com/files/udaq_snowchem_final_6aug15.pdf.

Fahey, K.M., Carlton, A.G., Pye, H.O., Baek, J., Hutzell, W.T., Stanier, C.O., Baker, K.R., Appel, K.W., Jaoui, M., Offenberg, J.H., 2017. A framework for expanding aqueous chemistry in the Community Multiscale Air Quality (CMAQ) model version 5.1. Geoscientific Model Development 10.

Fountoukis, C., Nenes, A., 2007. ISORROPIA II: a computationally efficient thermodynamic equilibrium model for K+-Ca2+-Mg2+-Nh(4)(+)-Na+-SO42--NO3--Cl--H2O aerosols. Atmospheric Chemistry and Physics 7, 4639-4659.

Goldberg, D.L., Lu, Z., Streets, D.G., de Foy, B., Griffin, D., McLinden, C.A., Lamsal, L.N., Krotkov, N.A., Eskes, H., 2019. Enhanced Capabilities of TROPOMI NO2: Estimating NO X from North American Cities and Power Plants. Environmental science & technology 53, 12594-12601.

Hu, X., Yu, C., Tian, D., Ruminski, M., Robertson, K., Waller, L.A., Liu, Y., 2016. Comparison of the Hazard Mapping System (HMS) fire product to ground-based fire records in Georgia, USA. Journal of Geophysical Research: Atmospheres 121, 2901-2910.

Hu, Y., Odman, M.T., Chang, M.E., Jackson, W., Lee, S., Edgerton, E.S., Baumann, K., Russell, A.G., 2008. Simulation of air quality impacts from prescribed fires on an urban area. Environmental Science & Technology 42, 3676-3682.

Jiang, X., Wiedinmyer, C., Carlton, A.G., 2012. Aerosols from fires: An examination of the effects on ozone photochemistry in the Western United States. Environmental Science & Technology 46, 11878-11886.

Kelly, J.T., Koplitz, S.N., Baker, K.R., Holder, A.L., Pye, H.O., Murphy, B.N., Bash, J.O., Henderson, B.H., Possiel, N.C., Simon, H., 2019. Assessing PM2. 5 model performance for the conterminous US with comparison to model performance statistics from 2007-2015. Atmospheric Environment 214, 116872.

Knepp, T.N., Szykman, J.J., Long, R., Duvall, R.M., Krug, J., Beaver, M., Cavender, K., Kronmiller, K., Wheeler, M., Delgado, R., 2017. Assessment of mixed-layer height estimation from single-wavelength ceilometer profiles. Atmospheric measurement techniques 10, 3963-3983.

Laing, J.R., Jaffe, D.A., Slavens, A.P., Li, W., Wang, W., 2017. Can d; PM2. 5/d; CO and d; NOy/d; CO Enhancement Ratios Be Used to Characterize the Influence of Wildfire Smoke in Urban Areas? Aerosol and Air Quality Research 17, 2413-2423.

Langford, A.O., Alvarez II, R.J., Kirgis, G., Senff, C.J., Caputi, D., Conley, S.A., Faloona, I.C., Iraci, L.T., Marrero, J.E., McNamara, M.E., 2019. Intercomparison of lidar, aircraft, and surface ozone measurements in the San Joaquin Valley during the California Baseline Ozone Transport Study (CABOTS). Atmospheric Measurement Techniques 12, 1889-1904.

Langford, A.O., Senff, C.J., Alvarez II, R.J., Aikin, K.C., Baidar, S., Bonin, T.A., Brewer, W.A., Brioude, J., Brown, S.S., Burley, J.D., 2021. The Fires, Asian, and Stratospheric Transport-Las Vegas Ozone Study (FAST-LVOS). Atmospheric Chemistry and Physics Discussions, 1-51.

Larkin, N.K., O'Neill, S.M., Solomon, R., Raffuse, S., Strand, T., Sullivan, D.C., Krull, C., Rorig, M., Peterson, J., Ferguson, S.A., 2010. The BlueSky smoke modeling framework. International Journal of Wildland Fire 18, 906-920.

Larkin, N.S.R., S.; Huang, S.; Pavlovic, N.; Rao, V., 2020. The Comprehensive Fire Information Reconciled Emissions (CFIRE) Inventory: Wildland Fire Emissions Developed for the 2011 and 2014 U.S. National Emissions Inventory (in press). Journal of the Air & Waste Management Association.

Li, Y., Tong, D., Ngan, F., Cohen, M., Stein, A., Kondragunta, S., Zhang, X., Ichoku, C., Hyer, E., Kahn, R., 2020. Ensemble PM2. 5 forecasting during the 2018 camp fire event using the HYSPLIT transport and dispersion model. Journal of Geophysical Research: Atmospheres 125, e2020JD032768.

Liu, Y., Achtemeier, G., Goodrick, S., Jackson, B., Qu, J., 2011. Evaluation and Improvement of Smoke Plume Rise Models.

Liu, Y., Kochanski, A., Baker, K.R., Mell, W., Linn, R., Paugam, R., Mandel, J., Fournier, A., Jenkins, M.A., Goodrick, S., 2019. Fire behaviour and smoke modelling: Model improvement and measurement needs for next-generation smoke research and forecasting systems. International journal of wildland fire 28, 570-588.

Loría-Salazar, S.M., Holmes, H.A., Arnott, W.P., Barnard, J.C., Moosmüller, H., 2016. Evaluation of MODIS columnar aerosol retrievals using AERONET in semi-arid Nevada and California, USA, during the summer of 2012. Atmospheric Environment 144, 345-360.

McClure, C.D., Jaffe, D.A., 2018. Investigation of high ozone events due to wildfire smoke in an urban area. Atmospheric Environment 194, 146-157.

Prichard, S., Larkin, N.S., Ottmar, R., French, N.H., Baker, K., Brown, T., Clements, C., Dickinson, M., Hudak, A., Kochanski, A., 2019. The Fire and Smoke Model Evaluation Experiment—A Plan for Integrated, Large Fire–Atmosphere Field Campaigns. Atmosphere 10, 66.

Prichard, S.J., O'Neill, S.M., Eagle, P., Andreu, A.G., Drye, B., Dubowy, J., Urbanski, S., Strand, T.M., 2020. Wildland fire emission factors in North America: synthesis of existing data, measurement needs and management applications. International Journal of Wildland Fire 29, 132-147.

Shrivastava, M., Cappa, C.D., Fan, J., Goldstein, A.H., Guenther, A.B., Jimenez, J.L., Kuang, C., Laskin, A., Martin, S.T., Ng, N.L., 2017. Recent advances in understanding secondary organic aerosol: Implications for global climate forcing. Reviews of Geophysics.

Simon, H., Bhave, P.V., 2012. Simulating the Degree of Oxidation in Atmospheric Organic Particles. Environmental Science & Technology 46, 331-339.

Skamarock, W.C., Klemp, J.B., Dudhia, J., Gill, D.O., Barker, D.M., Duda, M.G., Huang, X., Wang, W., Powers, J.G., 2008. A description of the Advanced Reserch WRF version 3. NCAR Technical Note NCAR/TN-475+STR.

U. S. Environmental Protection Agency, 2020. Policy Assessment for the Review of the Ozone National Ambient Air Quality Standards. EPA-452/R-20-001. https://www.epa.gov/naaqs/ozone-o3-standards-policy-assessments-current-review.

U.S. Environmental Protection Agency, 2016. Guidance on the Preparation of Exceptional Events Demonstrations for Wildfire Events that May Influence Ozone Concentrations. https://www.epa.gov/sites/default/files/2018-10/documents/exceptional_events_guidance_9-16-16_final.pdf.

Urbanski, S., 2014. Wildland fire emissions, carbon, and climate: Emission factors. Forest Ecology and Management 317, 51-60.

Van Der Werf, G.R., Randerson, J.T., Giglio, L., Van Leeuwen, T.T., Chen, Y., Rogers, B.M., Mu, M., Van Marle, M.J., Morton, D.C., Collatz, G.J., 2017. Global fire emissions estimates during 1997-2016.

Wiedinmyer, C., Akagi, S., Yokelson, R.J., Emmons, L., Al-Saadi, J., Orlando, J., Soja, A., 2011. The Fire INventory from NCAR (FINN): A high resolution global model to estimate the emissions from open burning. Geoscientific Model Development 4, 625.

Zhou, L., Baker, K.R., Napelenok, S.L., Pouliot, G., Elleman, R., O'Neill, S.M., Urbanski, S.P., Wong, D.C., 2018. Modeling crop residue burning experiments to evaluate smoke emissions and plume transport. Science of The Total Environment 627, 523-533.

APPENDIX A

Additional Details about the Photochemical Model Application

The CMAQ model version 5.3.2 was applied with ISORROPIA II inorganic thermodynamics (Fountoukis and Nenes, 2007), aqueous phase chemistry (Fahey et al., 2017), and gas phase chemistry based on the Carbon Bond 6 revision 3 mechanism (Emery et al., 2015). Primary organic aerosol is treated as non-volatile and secondary organic aerosol (SOA) was formed based on yields from precursor gases. This treatment conserves the POA mass and results in low SOA/POA ratios, which is consistent with most observations of ambient fire plumes, albeit the aging of the organic aerosol in the plumes is not captured (Cubison et al., 2011; Shrivastava et al., 2017). The ratio of organic mass to organic carbon is assumed to be 1.7 for wildland fire emissions (Simon and Bhave, 2012). Photolysis rates were attenuated in the presence of model predicted particulate matter (Baker et al., 2016).

Meteorological inputs to CMAQ were simulated with the WRF model version 4.1.1 (Skamarock et al., 2008). WRF and CMAQ were applied for the entire year of 2018 for a 12 km domain covering the contiguous U.S., southern Canada, and Mexico. Each model used 35 layers to represent the vertical atmosphere from the surface up to 50 mb. CMAQ was initialized with a hemispheric CMAQ model simulation which provided initial chemical conditions and also boundary inflow.

Anthropogenic emissions were based on the 2016 National Emission Inventory with year specific data used for point sources reporting continuous emissions data. Mobile emissions were projected from 2016 to 2018 to reflect reductions in emissions due to fleet turnover and implementation of control programs. Biogenic emissions were estimated with the Biogenic Emission Inventory System version 3.6.1 (Bash et al., 2015).

The impacts of different fire types were estimated using the brute-force differential method. A baseline simulation was done with all emissions sources and subsequent simulations were done where one component was removed. The difference between the baseline and simulation where one component was removed is considered the contribution in this assessment. The impacts of U.S. wildfire, U.S. prescribed fire, U.S. agriculture fires, and Canada and Mexico fires were estimated with this approach.

Wildland fire emissions outside the United States are estimated with the Fire INventory from NCAR (Wiedinmyer et al., 2011). The Satellite Mapping Automated Reanalysis Tool for Fire Incident Reconciliation version 2 (SmartFire2; SF2) and BlueSky Framework/Pipeline were used to estimate emissions in the United States from wildland fires. SF2 is an algorithm and database system that combines multiple sources of fire information and reconciles them into a unified GIS database. It reconciles fire data from satellite sensors and ground-based reports, thus drawing on the strengths of both data types while avoiding double-counting of fire events (Larkin et al., 2010; Larkin, 2020).

The BlueSky Framework estimates fuel type, fuel loading, fuel consumption, and emissions based on the location, type, and size information provided by SF2 for each wildland fire in the contiguous U.S. and Alaska. Fuel loading is based on the Fuel Characteristic Classification System (FCCS) module and fuel consumption is based on the CONSUME module. The BlueSky Framework generated emission factors for wildland fires. The legacy option in BlueSky is the Fire Emissions Production Simulator (FEPS). The Smoke Emissions Reference Application (SERA) described in (Prichard et al., 2020) is the most extensive

compilation of smoke emission factors for North American fires to date. Wildland fire emission factors were estimated using both the FEPS and SERA database (Prichard et al., 2020). These annual model simulations for 2018 used FEPS and SERA emissions factors for wildland fire emissions. The SERA emission factors might result in somewhat larger $PM_{2.5}$ impacts at times but would not change anything about seasonal timing associated with different fire types. Hypothetical wildfire modeling was done using SERA emission factors.

Daily emission estimates for each wildland fire are processed for input to photochemical models using the Sparse Matrix Operator Kernel Emissions (SMOKE; https://www.cmascenter.org/smoke/). SMOKE was used to apply a fire type-specific diurnal profile and allocates total emissions of nitrogen oxides, volatile organic compounds, and $PM_{2.5}$ to specific model species needed for chemical mechanisms. Speciation profiles are based on those available in the SPECIATE database (www.epa.gov/air-emissions-modeling/speciate).

United States Environmental Protection Agency

Office of Air Quality Planning and Standards
Air Quality Assessment Division
Research Triangle Park, NC

Publication No. EPA-454/R-22-002
March 2022