4   Chemical Tomography in a Fresh Wildland Fire Plume: a Large Eddy

5   Simulation (LES) Study

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31   **Contents of this file**

34

35   **Section S1. WRF-LES Technical Updates.**

36   The publicly released WRF v4.0 is used in this work. Several new updates have been
37   released in newer versions of WRF. Two of them are relevant for this work: (1) A bug fix that
38   improves the potential temperature tendency, which is recently implemented in WRF v4.2.2
39   (https://github.com/wrf-model/WRF/pull/1259/files#diff-
40   d6fd08d956dbe380e8c1094cfc668bd4); and (2) another bug fix that improves the momentum
41   flux and sub-grid scale stress, which is implemented in WRF v4.2.1 (https://github.com/wrf-
42   model/WRF/pull/1214/files/323fc93b19465163ef6529e79eec5a82292e5eb1). These two new
43   implementations are merged into the WRF model version 4.0 used in this work.

44   This idealized WRF-LES model is evaluated against another widely used LES model,
45   NCAR-LES (Patton et al., 2005). In this comparision, both WRF-LES and NCAR-LES are configured
46   in the same way (i.e., same initial conditions, driven by the same surface heat and moisture
47   fluxes). It drew our attention that the friction velocity (U_*) calculated using this WRF-LES (with
48   the aforementioned bug fixes) is roughly a factor of two lower than that calculated using NCAR-
49   LES. The reason may be that, in the default WRF, the friction velocity is calculated using the
50   bulk Richardson number, which may not be properly updated in idealized WRF-LES when the
51   surface heat flux is prescribed (personal communication: Jimy Dudhia, National Center for
52   Atmospheric Research). Therefore, a new friction velocity scheme is developed in this work for
53   the idealized WRF-LES to solve U_* directly:

54     $$U_* = \frac{\kappa U}{\ln(\frac{z}{z_0}) - \Psi_m(\frac{z}{L})}$$ Equation S1

55     $$L = -\frac{\rho C_p \theta U_*^3}{\kappa g H}$$ Equation S2

56   Where κ is the von Kármán constant, U is the surface horizontal wind speed (m s^{-1}), z_0 is the
57   roughness length scale (m), Ψ_m is the stability correction function for momentum (in the WRF
58   surface layer scheme), L is the Obukhov length (m), ρ is the air density (kg m^{-3}), C_p is the heat
59   capacity (1005 J kg^{-1} K^{-1}), ϑ is the potential temperature (K), H is the surface heat flux (W m^{-2}),
60   and g is the acceleration due to gravity (9.8 m s^{-2}),. Equations S1 and S2 are solved implicitly
61   using the Newton iteration method. Using this new scheme, the friction velocity calculated in
62   this idealized WRF-LES driven by surface heat fluxes is greatly improved and in very good
63   agreement with the NCAR-LES.

64   Other major physical and dynamical settings of the WRF-LES model are summarized as
65   follows: microphysics option: Morrison 2-moment scheme (mp_physics = 10);

66 longwave/shortwave radiation option: Rapid Radiative Transfer Model for GCMs (RRTMG;
67 ra_lw_physics/ra_sw_physics = 4); turbulence and mixing option: evaluates mixing terms in
68 physical space (stress form; diff_opt = 2); eddy coefficient option: 1.5 order TKE closure
69 (km_opt = 2).

70

71 **Section S2. Mesoscale WRF-Chem**

72   A mesoscale WRF-Chem simulation (12 km horizontal resolution) was used to generate
73 the initial conditions for the WRF-LES model (Figures S1 and S2). Some of the major settings of
74 this 12 km WRF-Chem simulation are summarized as follows: microphysics option: Morrison 2-
75 moment scheme (mp_physics = 10); longwave/shortwave radiation option: Rapid Radiative
76 Transfer Model for GCMs (RRTMG; ra_lw_physics/ra_sw_physics = 4); turbulence and mixing
77 option: evaluates mixing terms in physical space (stress form; diff_opt = 2); eddy coefficient
78 option: horizontal Smagorinsky first order closure (km_opt = 4); surface-layer option: MYNN
79 surface layer (sf_sfclay_physics = 5); land-surface option: Noah Land-Surface Model
80 (sf_surface_physics = 2); boundary-layer option: MYNN 2.5 level TKE scheme (bl_pbl_physics =
81 5); cumulus option: Grell-Devenyi ensemble scheme (cu_physics = 3); chemistry option:
82 NOAA/ESRL RACM chemical mechanism (chem_opt = 108); photolysis option: Madronich
83 photolysis (TUV; phot_opt = 1).

84

85 **Table S1.** The highly simplified chemical mechanism used in the WRF-LES model. This
86 mechanism is condensed based on T1 MOZART in the WRF package (Knote et al., 2014).

Reactions	Rate coefficients
O_3 = 2 OH	O3_hv_H2O(T, [M], [H2O], j_O1D), note 1
NO_2 + hv = NO + O_3	FTUV
NO_2 + aerosols = 0.5 HNO_2	$\gamma = 5 \times 10^{-4}$, note 2
HNO_2 + hv = OH + NO	FTUV
H_2O_2 + hv = 2 OH	FTUV
HCHO + hv = 2 HO_2 + CO	FTUV
HCHO + hv = CO	FTUV
OH + HO_2 = H_2O	T1 MOZART
OH + O_3 = HO_2	T1 MOZART
HO_2 + HO_2 = H_2O_2	T1 MOZART
HO_2 + O_3 = OH	T1 MOZART
NO + O_3 = NO_2	T1 MOZART
NO_2 + OH =	T1 MOZART
NO_2 + O_3 = NO_3	T1 MOZART
NO + HO_2 = NO_2 + OH	T1 MOZART
NO_2 + NO_3 = N_2O_5	T1 MOZART
NO + NO_3 = NO_2 + NO_2	T1 MOZART
HO_2 + NO_3 = OH + NO_2	T1 MOZART
N_2O_5 = NO_2 + NO_3	T1 MOZART
N_2O_5 =	T1 MOZART
NO_3 + hv = 0.11 NO + 0.89 NO_2 + 0.89 O_3	FTUV
CH_3O_2 + NO = HCHO + 0.99 NO_2 + HO_2	T1 MOZART
CH_3O_2 + HO_2 =	T1 MOZART
CO + OH = HO_2	T1 MOZART
CH_4 + OH = CH_3O_2	T1 MOZART
HCHO + OH = HO_2 + CO	T1 MOZART
C_3H_6 + OH = PO_2	T1 MOZART
PO_2 + NO = HO_2 + HCHO + ALDS + NO_2	T1 MOZART
PO_2 + HO_2 = POOH	T1 MOZART
POOH + OH = 0.5 PO_2 + 0.5 OH + 0.5 ALDS	T1 MOZART
C_3H_6 + O_3 = 0.5 HCHO + 0.5 ALDS + 0.28 CH_3O_2 + 0.28 HO_2 + 0.36 OH	T1 MOZART
C_3H_6 + NO_3 = NO_2 + ALDS	T1 MOZART
ISOP + OH = $ISOPO_2$	T1 MOZART
ISOP + O_3 = 0.6 MVKMACR + 0.27 OH + 0.06 HO_2 + 0.6 HCHO + 0.3 CO + 0.1 O_3 + 0.2 RCO_3	T1 MOZART, note 3
ISOP + NO_3 = $ISOPNO_3$	T1 MOZART
$ISOPO_2$ + NO = 0.08 ONITR + 0.92 NO_2 + 0.55 MVKMACR + 0.37 ALDS + 0.55 HCHO + HO_2	T1 MOZART
$ISOPO_2$ + HO_2 = ISOPOOH	T1 MOZART

Reaction	Reference
ISOPO2 + CH3O2 = HO2 + 1.2 HCHO + 0.45 MVKMACR + 0.3 ALDS	T1 MOZART
ISOPOOH + OH = 0.5 XO2 + 0.5 ISOPO2	T1 MOZART
ISOPOOH + hv = 0.69 MVKMACR + 0.69 HCHO + HO2	FTUV
MACRO2 + NO = NO2 + 0.47 HO2 + 0.25 HCHO + ALDS + 0.53 RCO3 + 0.22 CO	T1 MOZART
MACRO2 + HO2 =	T1 MOZART
MACRO2 + CH3O2 = 0.73 HO2 + 0.88 HCHO + 0.11 CO + 0.73 ALDS + 0.26 RCO3	T1 MOZART
MVKMACR + hv = 0.165 OH + 0.335 HO2 + 0.65 RCO3 + 0.335 HCHO + 0.685 CO + 0.15 CH3O2	T1 MOZART
MVKMACR + OH = 0.75 MACRO2 + 0.25 RCO3	T1 MOZART
MVKMACR + O3 = 0.75 HCHO + 0.895 ALDS + 0.148 OH + 0.2 O3 + 0.168 HO2 + 0.125 CO	T1 MOZART
ONITR + hv = HO2 + CO + NO2 + HCHO	T1 MOZART
ONITR + OH = ALDS + HO2 + 0.4 NO2	T1 MOZART
ALDS + OH = RCO3	T1 MOZART, note 4
ALDS + hv = CH3O2 + CO + HO2	j-CH3CHO in FTUV
XO2 + NO = NO2 + 1.5 HO2 + CO + 0.75 ALDS	T1 MOZART
XO2 + HO2 =	T1 MOZART
XO2 + CH3O2 = HO2 + 0.7 HCHO + 0.4 CO + 0.3 ALDS	T1 MOZART
RCO3 + NO = NO2 + HCHO	T1 MOZART
RCO3 + HO2 = 0.25 O3	T1 MOZART
RCO3 + CH3O2 = 2 HCHO + HO2	T1 MOZART
RCO3 + NO2 = PAN	T1 MOZART
PAN = RCO3 + NO2	T1 MOZART
PAN + hv = 0.8 RCO3 + 0.8 NO2 + 0.2 CH3O2 + 0.2 NO3	j-PAN in FTUV
ISOPNO3 + NO = 1.206 NO2 + 0.794 HO2 + 0.072 HCHO + 0.206 MVKMACR + 0.794 ONITR	T1 MOZART
ISOPNO3 + HO2 = 0.206 NO2 + 0.206 OH + 0.206 HCHO + 0.206 MVKMACR + 0.794 ONITR	T1 MOZART
BENZENE + OH = 0.83 HO2 + 0.18 CO + 0.35 BENZO2	T1 MOZART
BENZO2 + HO2 = BENZOOH	T1 MOZART
BENZO2 + NO = NO2 + 0.5 ALDS + HO2	T1 MOZART
BENZOOH + OH = BENZO2	T1 MOZART
TOLUENE + OH = 0.65 TOLO2 + 0.05 RCO3 + 0.38 HO2 + 0.15 CO	T1 MOZART
TOLO2 + HO2 = TOLOOH	T1 MOZART
TOLO2 + NO = NO2 + 0.6 ALDS + HO2	T1 MOZART
TOLOOH + OH = TOLO2	T1 MOZART
FURAN + OH = 0.39 DIAL + 0.49 HO2 + 0.51 FURANO2	Coggon et al., 2019
DIAL + OH = DIALO2	Coggon et al., 2019
DIALO2 + NO = NO2 + 0.49 MALANHY + 0.96 HO2 + 0.04 CH3O2	Coggon et al., 2019
DIALO2 + NO2 =	Coggon et al., 2019
DIAL + hv = 0.74 DIALO2 + 0.74 HO2 + 0.34 CO	$0.098*j_{NO2}$, Coggon et al., 2019

FURANO2 + NO = NO2 + FURANONE + 0.81 HO2 + 0.19 CH3O2	Coggon et al., 2019
FURANONE + OH = 0.69 MALANHY + 0.66 HO2 + 0.34 CH3O2 + 0.43 CO	Coggon et al., 2019
FURAN + O3 =	Coggon et al., 2019
FURAN + NO3 =	Coggon et al., 2019

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88 Note 1: O3_hv_H2O(T, [M], [H2O], j_O1D) = 1.63E-10*EXP(60/T)*[H2O]* j_O1D / (1.63E-10*EXP(60/T)*
89 [H2O] + 2.15E-11*EXP(110/T)*0.79*[M] + 3.30E-11*EXP(55/T)*0.21*[M]), where T is temperature (K),
90 and [M] and [H2O] are air and water vapor concentrations (molecules cm^{-3}), respectively. This approach
91 assumes steady-state for O^1D.

92 Note 2: the reactive uptake coefficient of NO2 is estimated from based on the literature values
93 (Ammann et al., 2013). Aerosol surface area in this work considers only BC and OC.

94 Note 3: MVKMACR is the sum of MVK and MACR.

95 Note 4: ALDS is a lumped species for aldehydes including acetaldehyde, glycolaldehyde, hydroxyacetone,
96 as well as lumped unsaturated hydroxycarbonyl from T1 MOZART. Of all these lumped species,
97 acetaldehyde is the most dominant one in fire plumes, therefore the kinetics of acetaldehyde (e.g.,
98 photolysis frequency, OH rate coeffcieint) are used for the removal of ALDS.

99

100   **Table S2.** Fire emissions used in the WRF-LES model. These emissions are adjusted until
101   reasonable agreements are achieved when compared to airborne measurements (Figure 3).

Species	Fire emission	Unit
NO	1097	ppb m s^{-1}
CO	77780	ppb m s^{-1}
ISOP	238	ppb m s^{-1}
MVKMACR	153	ppb m s^{-1}
EC	297	µg m^{-2} s^{-1}
OC	19649	µg m^{-2} s^{-1}
C3H6	802	ppb m s^{-1}
ALDS	560	ppb m s^{-1}
HNO2	123	ppb m s^{-1}
HCHO	930	ppb m s^{-1}
TOLUENE	129	ppb m s^{-1}
BENZENE	259	ppb m s^{-1}
FURAN	387	ppb m s^{-1}

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104 **Table S3.** NASA DC-8 airborne measurements used in this work. The NASA Langley Research
105 Center Online Custom Data Merging Tool (beta 1.4, https://www-air.larc.nasa.gov/cgi-
106 bin/Driver.cgi?operation=doMerge) is used to generate the 1-Hz merge dataset, except for the
107 DIAL data.

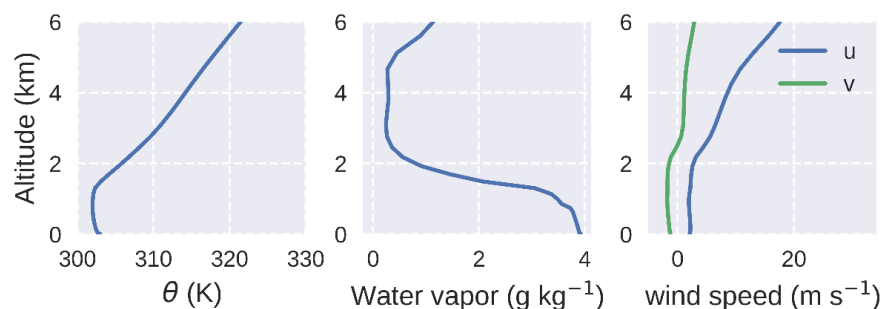| Measurements	Instrument	Reference
532 nm backscatter ratio	NASA Differential Absorption LIDAR (DIAL)	(Hair et al., 2008)
Ozone (O_3), nitrogen oxides (NO_x)	NOAA NOyO3 4-channel chemiluminescence	(Ryerson et al., 2000)
Photolysis frequencies (j-values)	NCAR CCD Actinix Flux Spectroradiometers (CAFS)	(Shetter & Müller, 1999)
Carbon monoxide (CO)	NASA Differential Absorption Carbon monOxide Measurement (DACOM)	(Warner et al., 2010)
Nitrous acid (HONO)	NOAA Iodide Time-of-Flight Chemical Ionization Mass Spectrometer (ToF CIMS)	(Neuman et al., 2016; Veres et al., 2020)
Peroxyacetyl nitrate (PAN)	GeorgiaTech chemical ionization mass spectrometer (CIMS)	(Huey, 2007)
Formaldehyde (HCHO)	NASA In Situ Airborne Formaldehyde (ISAF)	(Cazorla et al., 2015)
Black carbon (BC)	NOAA Single-Particle Soot Photometer (SP2)	(Schwarz et al., 2006)
Organic aerosol (OA), Organic Aerosol-to-organic carbon ratio (OA/OC Ratio)	CU High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-AMS)	(DeCarlo et al., 2006)
Ethane	CU Compact Atmospheric Multispecies Spectrometer (CAMS)	(P. Weibring et al., 2006; Petter Weibring et al., 2007)
Propane, i-butane, n-butane, i-pentane, n-pentane, i-butene/1-butene, isoprene, MVK, MACR, MEK, furan, 2-methylfuran,3-methylfuran, furfural	NCAR Trace Organic Gas Analyzer (TOGA)	(Apel et al., 2015; Wang et al., 2019)
Benzene, toluene, acetaldehyde, methanol, ethanol, acrolein, acetone/propanal, maleic anhydride, phenol, styrene	NOAA Proton-Transfer Reaction Time-of-Flight Mass Spectrometry (PTR-ToF-MS)	(Yuan et al., 2016)

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Figure S1. The vertical profiles of potential temperature (θ), water vapor, and wind used to initialize the LES model. These profiles are derived from the 12-km mesoscale WRF-Chem simulation (Section S2).
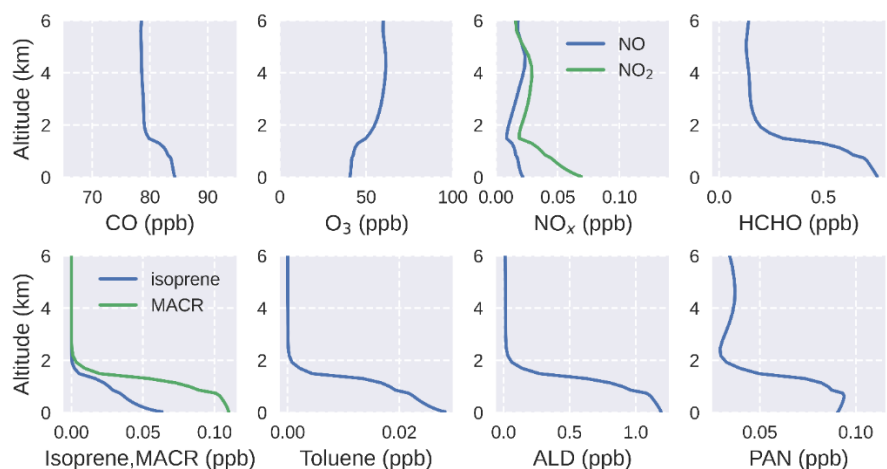

Figure S2. The vertical profiles of chemicals used to initialize the LES model. These profiles are derived from the 12-km mesoscale WRF-Chem simulation (Section S2).
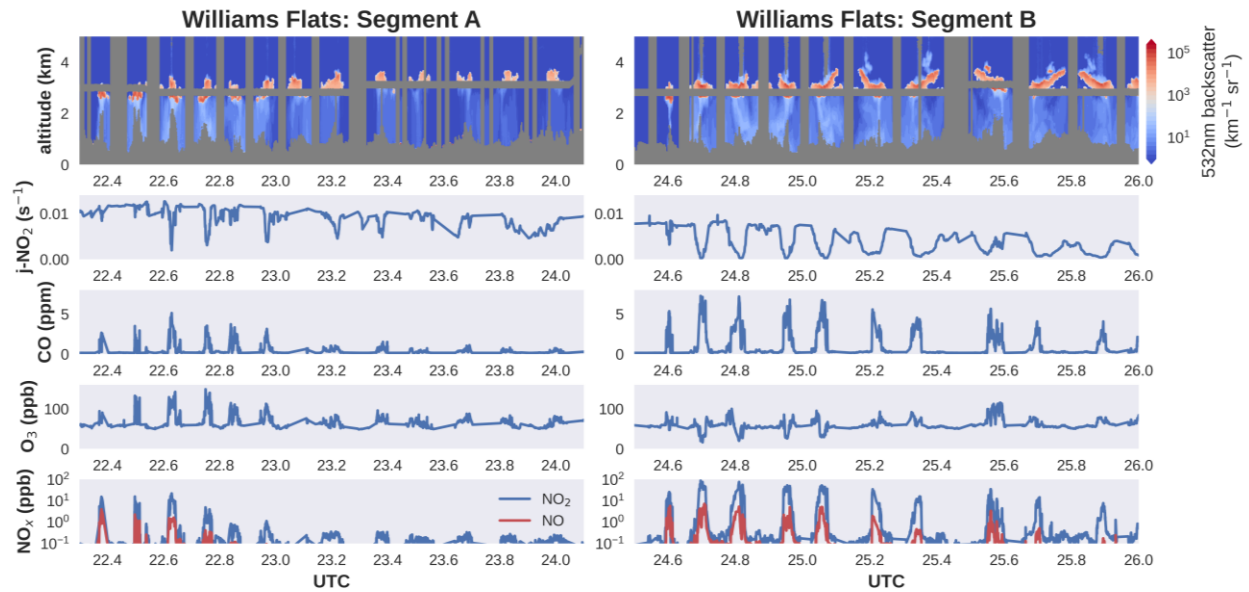
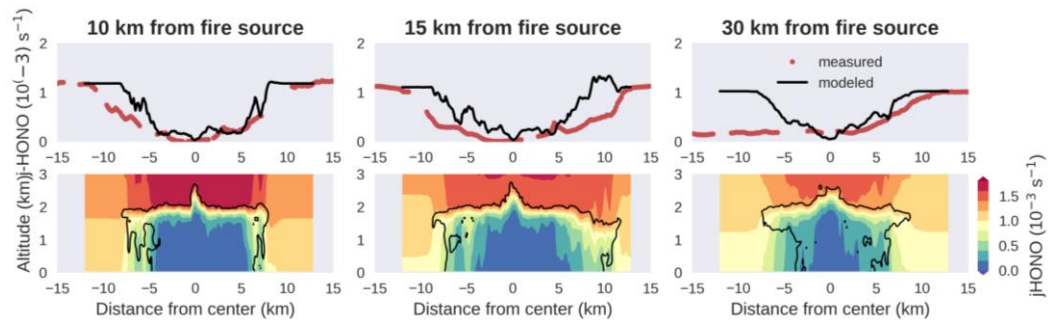Figure S3. Selected airborne measurements collected during the "in-plume" Segments A and B.

Figure S4. Measured j-HONO (top) during Segment B and modeled j-HONO across sections (bottom) at 10 km, 15 km, and 30 km downwind of the fire source. Also shown in the top panel are the modeled j-HONO sampled at the same distance from the fire, at 2 km above the model surface.
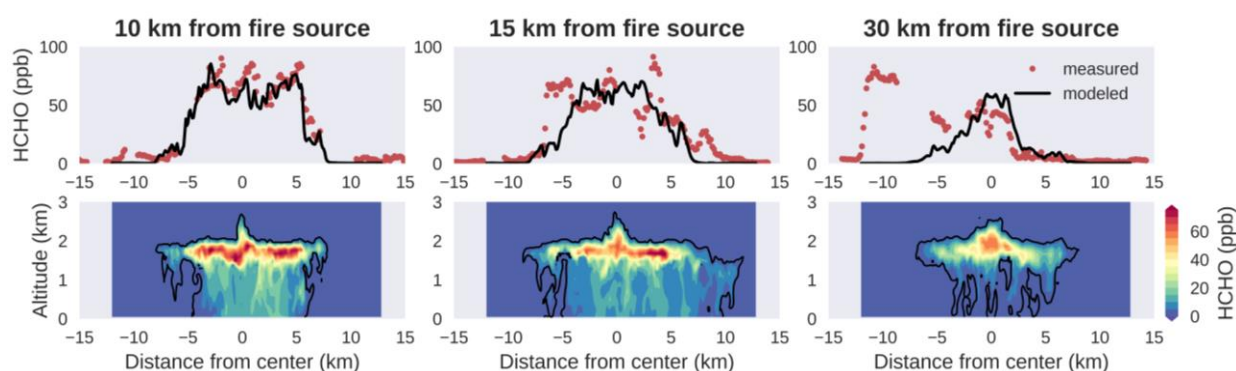
Figure S5. Same as Figure S4 but for NO_x.
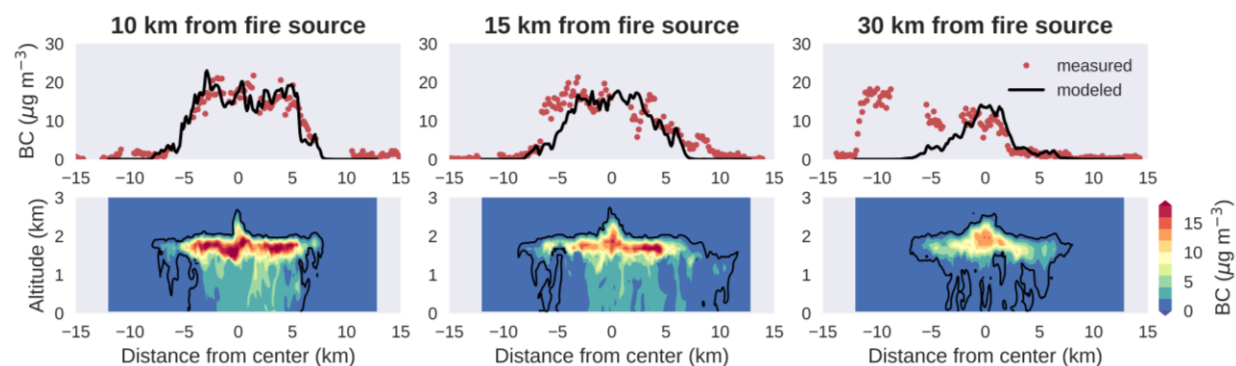

Figure S6. Same as Figure S4 but for HCHO.

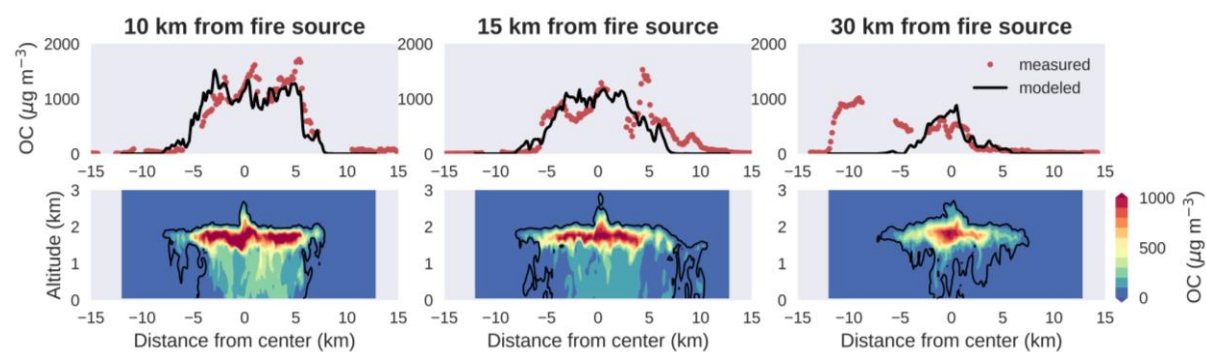Figure S7. Same as Figure S4 but for BC.

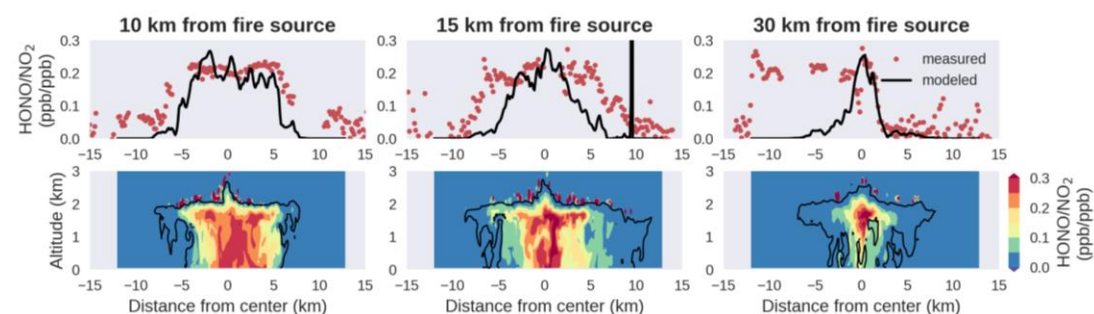Figure S8. Same as Figure S4 but for OC. OC is calculated from CU HR-AMS measured OA and OA/OC Ratio.

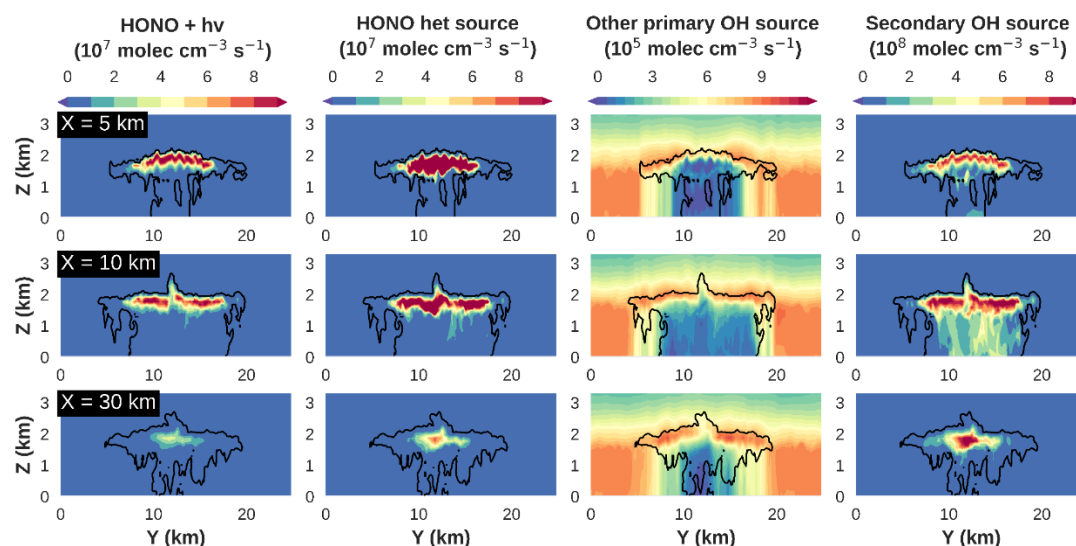Figure S9. Same as Figure S4 but for the ratio between HONO and NO_2 (ppb ppb^{-1}).

Figure S10. Modeled plume cross sections of HONO photolysis, heterogeneous HONO production, other primary OH source (mostly photolysis of O_3 and aldehydes), and secondary OH source, at X = 5, 10, and 30 km.
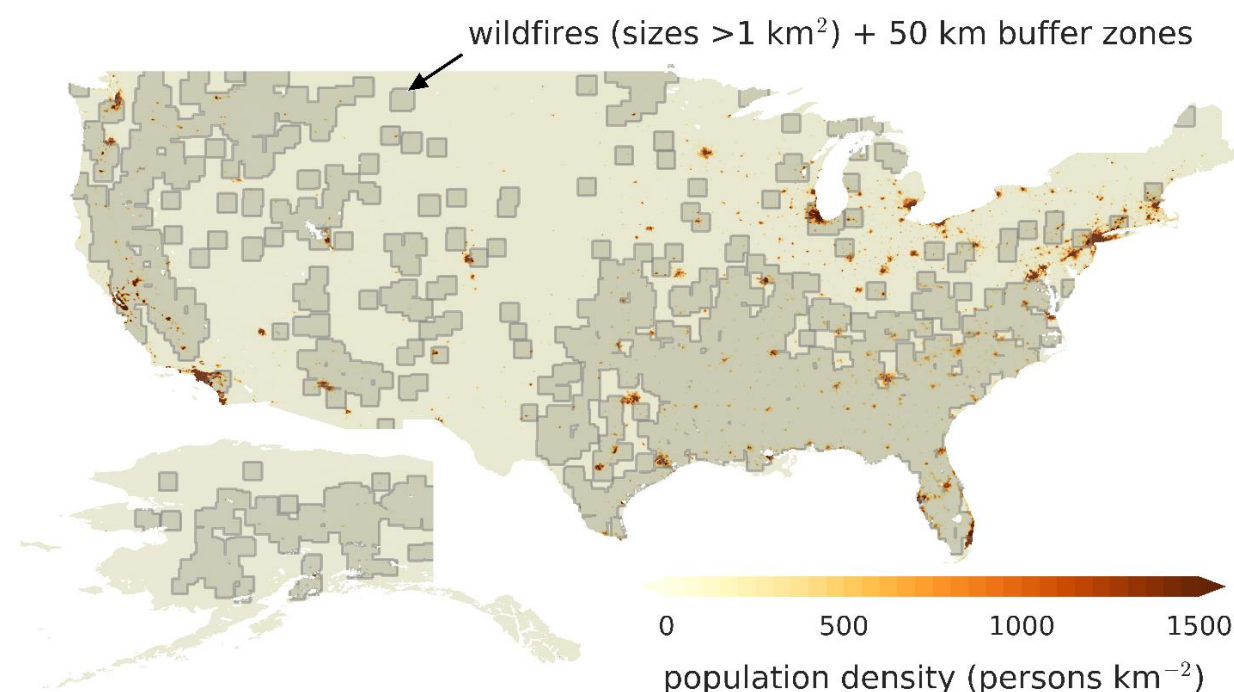

Figure S11. U.S. wildfires in 2019 larger than 1 km^2 (fire size) with 50 km buffer zones (grey patches) overlaid on the U.S. population density map. The wildfire sizes are reported in FINN version 2. The gridded U.S. population density map is from (Center for International Earth Science Information Network, Columbia University, 2020).

160

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