

Stratospheric intrusion-influenced ozone air quality exceedances investigated in the NASA MERRA-2 Reanalysis

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Key Points:

- NASA's MERRA-2 reanalysis is a publicly-available, high resolution (~ 50 km) dataset
- The MERRA-2 reanalysis, with assimilated O_3 , captures the fine-scale features of stratospheric intrusions known to impact surface air quality
- The combination of meteorological variables and O_3 may provide a valuable and unique tool for air quality managers

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Abstract

Stratospheric intrusions have been the interest of decades of research for their ability to bring stratospheric ozone (O_3) into the troposphere with the potential to enhance surface O_3 concentrations. However, these intrusions have been misrepresented in models and reanalyses until recently, as the features of a stratospheric intrusion are best identified in horizontal resolutions of 50 km or smaller. NASA’s Modern-Era Retrospective Analysis for Research and Applications Version-2 (MERRA-2) reanalysis is a publicly-available high-resolution dataset (~ 50 km) with assimilated O_3 that characterizes O_3 on the same spatiotemporal resolution as the meteorology. We demonstrate the science capabilities of the MERRA-2 reanalysis when applied to the evaluation of stratospheric intrusions that impact surface air quality. This is demonstrated through a case study analysis of stratospheric intrusion-influenced O_3 exceedences in spring 2012 in Colorado, using a combination of observations, the MERRA-2 reanalysis and the Goddard Earth Observing System Model, Version 5 (GEOS-5) simulations.

1 Introduction

Surface ozone (O_3) is harmful to human health and agriculture [Scherrer *et al.*, 2006; Krzyzanowski and Cohen, 2008]. Near the surface, O_3 is termed a secondary pollutant since it is a product of the photochemical reaction with precursors such as nitrogen oxides (NO_x ; NO and NO_2), carbon monoxide (CO) and non-methane hydrocarbons which have both man-made and natural emission sources in the troposphere. Therefore, in order to reduce near surface O_3 concentrations, communities must reduce anthropogenic pollution sources. However, the injection of stratospheric O_3 into the troposphere, known as a stratospheric intrusion (SI), can also lead to concentrations of ground-level O_3 exceeding the national ambient air quality standard (NAAQS) set by the Environmental Protection Agency (EPA), especially at high elevations [e.g., Langford *et al.*, 2009, 2015; Lin *et al.*, 2012, 2014; Yates *et al.*, 2013; Zhang *et al.*, 2014]. In October 2015, the EPA revised the US NAAQS for daily maximum 8-hour average (MDA8) O_3 from 75 parts per billion by volume (ppbv) to 70 ppbv [U.S. Environmental Protection Agency, 2015]. Therefore, it is crucial that we are able to understand, model, and predict SIs and their potential impact on surface O_3 concentrations.

SIs form as a result of the tropopause being drawn down below the jet stream, referred to as tropopause folding, often associated with an upper-level trough. SIs are characterized by O_3 -rich [e.g., Danielsen, 1968; Shapiro, 1974, 1980; Holton *et al.*, 1995; Browning, 1997] and CO-poor [Fischer *et al.*, 2000] air, with relatively high levels of potential vorticity (PV) [Holton *et al.*, 1995] and low levels of water vapor often observed in satellite imagery as a “dry slot” [e.g., Bader *et al.*, 1995; Wimmers *et al.*, 2003]. Therefore, tropopause folds can lead to the mixing of stratospheric and tropospheric air with different chemical and meteorological properties at low altitudes [e.g., Danielsen, 1980; Shapiro, 1980; Holton *et al.*, 1995], remaining behind a mid-latitude cyclone’s surface cold front [Browning, 1997; Bethan *et al.*, 1998; Cooper *et al.*, 2001; Knowland *et al.*, 2015]. The west coast of the USA is located at the end of the Pacific Ocean storm track [e.g. Hoskins and Hodges, 2002], a region favorable for stratosphere-to-troposphere transport of O_3 [James *et al.*, 2003; Sprenger and Wernli, 2003; Stohl *et al.*, 2003; Škerlak *et al.*, 2014]. On the lee-side of the Rocky Mountains, cyclones form (or redevelop) supported by upper-level troughs [McClain, 1960; Carlson, 1991]. However, the descending motion associated with the upper-level trough can still be a strong feature in the troposphere over the Rocky Mountains, prior to the identification of a surface low pressure system. In the upper-level flow, the troughs can form closed lows and even become “cut-off” from the westerly flow [Palmén and Newton, 1969]. This can result in the prolonged influence of the tropopause folds on tropospheric O_3 concentrations over a region [Lin *et al.*, 2012; Yates *et al.*, 2013] until the cut-off low (COL) dissipates or is reabsorbed into the mean flow [Nieto *et al.*, 2008]. During the winter and spring, there is a build-up of O_3 in the lower

69 stratosphere, and this leads to SIs having the largest influence on surface O₃ in the spring
70 [Danielsen and Mohnen, 1977; Holton et al., 1995; Monks, 2000].

71 For over 40 years, studies have observed the injection of O₃-rich air into the tropo-
72 sphere within tropopause folds over western USA [e.g., Lovill, 1970; Shapiro, 1980;
73 Langford et al., 1996, 2009, 2012; Wimmers et al., 2003; Cooper et al., 2004; Lefohn et al.,
74 2011] with recent studies focusing on the impact of SIs on O₃ air quality exceedences in
75 the high elevation communities of the Rocky Mountains [e.g., Langford et al., 2009, 2015;
76 Lin et al., 2012, 2014; Yates et al., 2013; Zhang et al., 2014]. Langford et al. [2009] fo-
77 cused on the transport of stratospheric O₃ in Colorado’s Front Range during the spring
78 of 1999 using lidar and surface measurements of O₃. They identified high concentrations
79 of O₃ in the mid-troposphere down to the surface as a result of tropopause folds asso-
80 ciated with upper-level troughs in the region. Lin et al. [2012] utilized the abundance
81 of vertical observations from ozonesondes and lidar taken during the 2010 NOAA Cal-
82 Nex field campaign in California as well as ground-based measurements throughout west-
83 ern USA, in conjunction with a model study to quantify the stratospheric fraction of air
84 that impacts NAAQS exceedence events. Using the NOAA Geophysical Research Lab-
85 oratory (GFDL) Atmosphere Model version 3 (AM3) with fully coupled stratosphere-
86 troposphere chemistry at ~50 km resolution, Lin et al. [2012] attributed 50–60 % of total
87 modelled surface O₃ in spring 2010 (as much as 20–40 ppbv of additional O₃ during
88 4 deep intrusions) to stratospheric origins on exceedence days. Using a coarser resolu-
89 tion model (~200 km), Lin et al. [2015] extended the analysis to April and May during
90 a 23-year period (1990–2012) and found the average stratospheric O₃ contribution is 15–
91 25 ppbv of western US surface O₃.

92 While the impact of SIs on surface O₃ in the western US is well documented, sim-
93 ulating and predicting such events remains challenging. The resolutions of current global
94 meteorological analyses (~10–50 km) are sufficient for resolving the dynamical evolution
95 of SIs, however these models typically contain very limited representations of trace gases
96 like O₃. Reanalyses have been used in numerous studies to explore the frequency, spa-
97 tial variations and structure of SIs [e.g., Stohl and Trickl, 1999; Waugh and Polvani, 2000;
98 Sprenger and Wernli, 2003; Lefohn et al., 2011; Reutter et al., 2015; Nath et al., 2016],
99 however, there are very few such studies which also use reanalysis O₃ [Škerlak et al., 2014;
100 Zanis et al., 2014; Knowland et al., 2015, 2017; Ott et al., 2016; Ryoo et al., 2017]. It
101 is our objective to investigate whether NASA’s Modern-Era Retrospective Analysis for
102 Research and Applications Version-2 (MERRA-2) reanalysis, which is similar to NASA’s
103 Global Modeling and Assimilation Office (GMAO) operational forecasting system, is able
104 to capture the dynamical features of a SI, in particular the isentropic descent of elevated
105 O₃ within and below the tropopause fold. Such datasets would support air quality agen-
106 cies for more rapid identification of the impact of stratospheric air on ground-level O₃
107 [Kaldunski et al., 2017] separate from local sources or the long-range transport of O₃ [Ryoo
108 et al., 2017]. The focus of this study will be on springtime (March - June (MAMJ)) O₃
109 air quality exceedences in 2012 which were identified by the EPA as having direct con-
110 nection with SIs [US EPA AQS database, 2017].

111 2 Data

112 2.1 Observational datasets

113 In the spring of 2012, there were seven days when the MDA8 O₃ [EPA AirData,
114 2016] at the Rocky Mountain National Park (RMNP) Long’s Peak monitoring station
115 (40.27°N, 105.54°W, 2742 m, Air Quality System (AQS) Site ID 08-069-0007, located
116 ~100 km northwest of Denver) exceeded the NAAQS of 75 ppbv as a result of SIs [US
117 EPA AQS database, 2017]: March 26th, April 6th, April 27th, May 26–28th, and June
118 14th. Several other suburban and rural monitoring stations in Colorado also reported
119 exceedences related to SIs on these and other dates in spring 2012 [US EPA AQS database,

120 2017]. Less than half of the diurnal variation in the hourly MAMJ O₃ at RMNP can be
 121 explained by the 1st (diurnal) harmonic, therefore other drivers in the O₃ variability must
 122 be considered. Deep SIs, those which impact surface O₃ concentrations, were anomalously
 123 frequent in the western USA in the spring of 2012 compared to the 1990–2012 period [*Lin*
 124 *et al.*, 2015], and observed MDA8 O₃ was also found to have a maximum in the west-
 125 ern USA that spring for the period 2004–2012 [*Baylon et al.*, 2016]. This study will ex-
 126 plore the representation of two of the SIs in remote sensing observations and the God-
 127 dard Earth Observing System Model, Version 5 (GEOS-5) model and assimilation prod-
 128 ucts. The first case study in early spring (March 26th local time (LT; +07:00 UTC) here-
 129 after will be referred to as the SI-1 event and the second case study, which occurred in
 130 late spring (May 26–28th event LT), will be referred to as the SI-2 event.

131 Daily total column O₃ (TCO) and relative humidity (RH) from the Atmospheric
 132 Infrared Sounder (AIRS) on NASA’s Aqua satellite are used to identify the presence of
 133 SIs over RMNP in observational data and to validate MERRA-2 reanalysis TCO since
 134 the AIRS O₃ data were not assimilated in MERRA-2. AIRS is equipped to measure both
 135 meteorological variables and chemical profiles [*Aumann et al.*, 2003; *Susskind et al.*, 2006;
 136 *Chahine et al.*, 2006] and observes the surface twice daily (01:30 and 13:30 LT). The re-
 137 trievals are performed even when clouds are present which makes the dataset ideal when
 138 analyzing regions near mid-latitude cyclones. The AIRS team produces several datasets
 139 of different spatiotemporal resolution. We use the level 3 version 6 (L3 V6) at 1° hor-
 140 izontal resolution [*AIRS Science Team/Joao Teixeira*, 2013].

141 2.2 Model datasets

142 NASA’s MERRA-2 reanalysis is an ideal candidate to explore the vertical struc-
 143 ture of the SIs over RMNP as it is a publicly-available, high-resolution reanalysis dataset
 144 (0.5° x 0.625° latitude-by-longitude grid, nominally ~50 km in the latitudinal direction,
 145 72 model layers up to 0.01 hPa [*Bosilovich et al.*, 2016; *Gelaro et al.*, 2017]) which as-
 146 similates both O₃ and meteorological observations [*Bosilovich et al.*, 2015; *McCarty et al.*,
 147 2016; *Gelaro et al.*, 2017]. The MERRA-2 reanalysis covers the period from January 1,
 148 1980 to within a couple weeks of real time and is the product of the GEOS-5 data as-
 149 similation system (DAS) [*Bosilovich et al.*, 2015; *Gelaro et al.*, 2017]. The GEOS-5 model
 150 includes monthly-averaged ozone production and loss rates linearly interpolated to daily
 151 values for both the stratosphere and the troposphere [*Bosilovich et al.*, 2016]. After 2004,
 152 MERRA-2 assimilates satellite retrievals of TCO from the Ozone Monitoring Instrument
 153 (OMI; *Levelt et al.* [2006]) and stratospheric O₃ profiles from the Microwave Limb Sounder
 154 (MLS; *Waters et al.* [2006]) [*Bosilovich et al.*, 2015; *McCarty et al.*, 2016; *Gelaro et al.*,
 155 2017]. MERRA-2 O₃ in the lower stratosphere is well-represented and has been shown
 156 to agree with ozonesondes [*Wargan et al.*, 2015, 2017]; therefore, where there is direct
 157 influence of stratospheric O₃ into the troposphere, such as an SI, we can expect realis-
 158 tic intrusions although possibly biased since the background ozone in the troposphere
 159 is simulated by simple chemistry parametrization [*Ott et al.*, 2016].

160 The meteorological and chemical variables – winds (u, v), vertical velocity (ω), equiv-
 161 alent potential temperature (θ_e ; calculated from temperature and specific humidity), Er-
 162 tel’s PV (EPV), RH and O₃ mixing ratios – were extracted on pressure levels up to 150
 163 hPa [*GMAO*, 2015a]. In addition, MERRA-2 sea-level pressure (SLP) [*GMAO*, 2015b]
 164 and TCO [*GMAO*, 2015c] are used in the comparison to the AIRS retrievals.

165 Two additional model variables are used: GEOS-5 simulated CO using emissions
 166 described in *Ott et al.* [2010] and an idealized stratospheric “influence” tracer (STFR)
 167 from *Ott et al.* [2016]. The STFR is set to 1 in the stratosphere and to 0 at the surface.
 168 For the STFR simulation, the tropopause was the higher height of the thermal tropopause
 169 or the dynamical tropopause. In the GEOS model, the dynamical tropopause is defined

170 as the 3 PVU isosurface, where 1 PV unit (PVU) = 10^{-6} K m² kg⁻¹ s⁻¹, which is higher
171 than the conventional 2 PVU isosurface [Holton *et al.*, 1995].

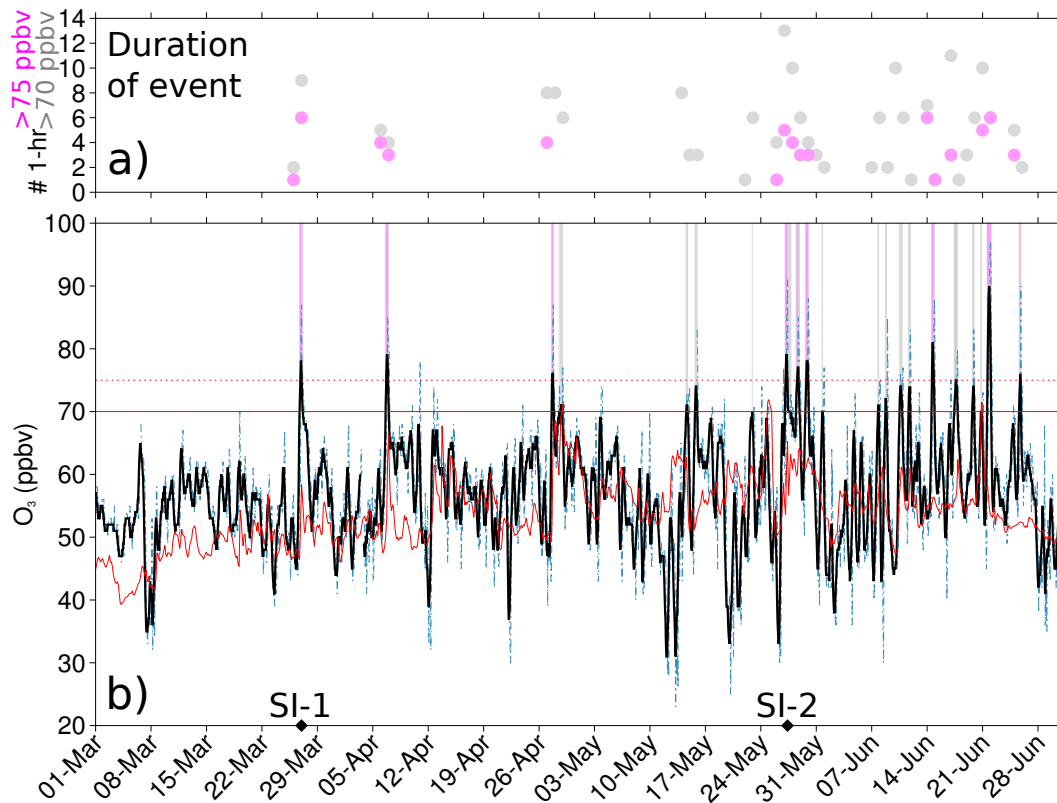
172 3 Results

173 The 8-hour running average O₃ and the hourly average O₃ observed at RMNP and
174 the corresponding 3-hourly surface O₃ from MERRA-2 [GMAO, 2015d] are presented
175 here for spring of 2012 (Fig. 1b). During the SI-1 event, the observed hourly O₃ at RMNP
176 ≥ 75 ppbv for 7 hours (1 hour March 26th and 6 hours March 27th, based on UTC, Fig. 1a)
177 with the maximum observed hourly O₃ equal to 87 ppbv observed at March 27, 2012 00UTC
178 (Fig. 1b; MERRA-2 O₃ = 58 ppbv). The second intrusion event, SI-2, influenced ground-
179 level O₃ for several days at RMNP; observed hourly O₃ ≥ 75 ppbv for 11 hours during
180 this 3-day period (Fig. 1a) with maximum observed hourly O₃ of 91 ppbv at 09 UTC
181 on May 27, 2012 (Fig. 1b; MERRA-2 O₃ = 65 ppbv). Considering the new NAAQS value
182 for MDA8 O₃, RMNP observed hourly O₃ ≥ 70 ppbv for 11 hours during the SI-1 event
183 and 30 hours for the SI-2 event (Fig. 1a). Figure 1 highlights the doubling of possible
184 exceedence days if the new MDA8-O₃ NAAQS of ≥ 70 ppbv is applied to 2012. As ex-
185 pected, the MERRA-2 surface O₃ for the grid box closest to RMNP underestimates the
186 O₃ variability of a point source measurement ($r^2 = 0.34$, based on 968 3-hourly timesteps;
187 Fig. 1b) in part because of the simple O₃ chemistry in the GEOS-5 model; however, there
188 are spikes in the reanalysis O₃ at or near the times of observed O₃ exceedences, portray-
189 ing the influence of stratospheric O₃ on the grid-box.

210 At the time of an intrusion, relatively dry air is expected to descend toward the
211 surface behind a cold front [e.g., Bethan *et al.*, 1998; Cooper *et al.*, 2001; Knowland *et al.*,
212 2015]. Due to the topography, SLP over the Rocky Mountains can be difficult to inter-
213 pret, however both of the SI case studies occurred when there was a low pressure in the
214 Northern Plains region (Fig. 2a,c). During the SI-1 event, there were two low pressure
215 systems, one in southwest Montana and one in southeast Wyoming (Fig. 2a). The 700 hPa RH
216 was low to the west of a surface trough extending from Wyoming approximately due south
217 into Mexico. For the late spring SI-2 event, a cyclone tracked northeastward into North
218 Dakota with a cold front trailing into western Kansas where it transitions to a station-
219 ary front (Fig. 2c). Here, a new low pressure system formed in southeastern Colorado,
220 from which a dry line extends southward through Texas. While relatively low RH is ob-
221 served by AIRS to the west of the cold front through the Dakotas and Nebraska, there
222 is an even stronger gradient in RH across the dry line (Fig. 2c).

223 The SI events can be identified by concurrent observations of O₃-rich air with the
224 low RH. This can be achieved by focusing on regions where the gradients in TCO are
225 large [Olsen *et al.*, 2000; Ott *et al.*, 2016]. The spatial distributions in AIRS TCO and
226 MERRA-2 TCO at the approximate time of the AIRS observations agree well [Ott *et al.*,
227 2016], although the MERRA-2 TCO is generally biased low compared to observations
228 in Fig. 2b,d. This aligns with the findings of Wargan *et al.* [2017] that MERRA-2 TCO
229 in the mid-latitudes was biased low compared to independent TCO measurements from
230 the TOMS (Total Ozone Mapping Spectrometer; Herman *et al.*, 1991) instrument. The
231 maximum TCO – in both AIRS and MERRA-2 – stretches from the Pacific Northwest
232 into the Rocky Mountain states linearly in Fig. 2b and with curvature in Fig. 2d. The
233 location of large TCO gradients in Fig. 2b,d correspond to the low RH regions in Fig. 2a,c;
234 in particular, large TCO gradients in both AIRS and MERRA-2 and low RH are co-located
235 over Colorado (Fig. 2).

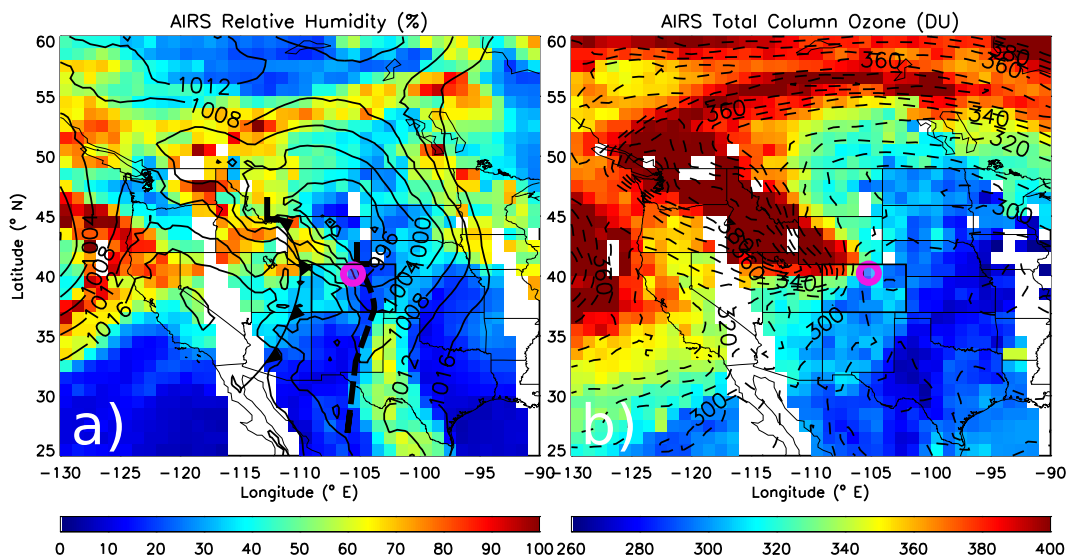
236 We look for further evidence of the SI-1 and SI-2 tropopause folding events in the
237 MERRA-2 reanalysis at the time of maximum O₃ at RMNP (Fig. 3). From 300 to 500 hPa
238 over the western USA, there are fine-scale filaments of stratospheric air, specifically high
239 levels of O₃ within the 2 PVU contour, which distinguish the SI events from the back-
240 ground (Fig. 3). At the time of maximum hourly O₃ observed at RMNP during the SI-1



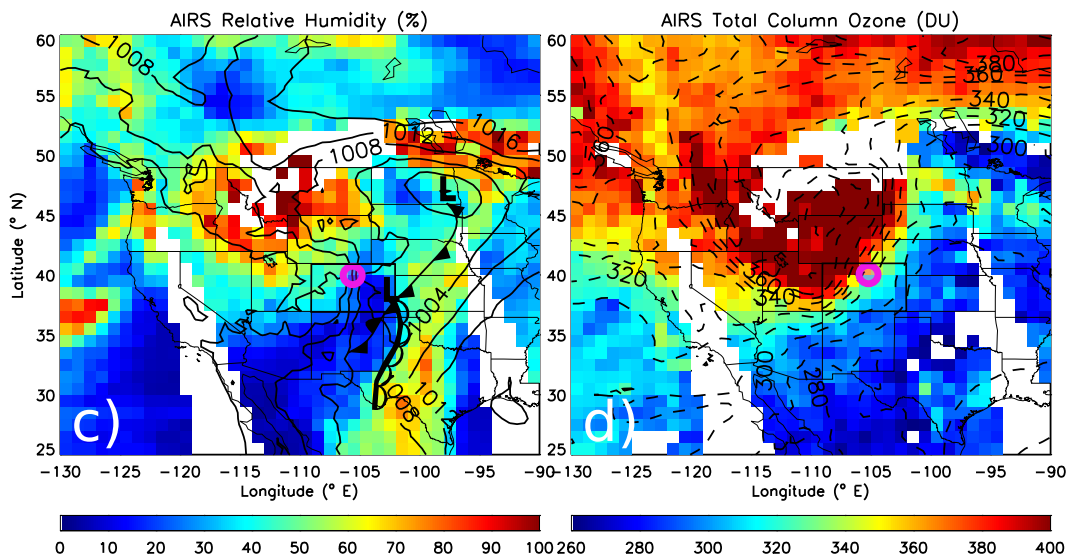
190 **Figure 1.** **a)** Number of hours in an exceedence day (time in UTC) where the RMNP ob-
 191 served hourly average $O_3 \geq 75$ ppbv (pink circles) and ≥ 70 ppbv (grey circles) **b)** 8-hourly
 192 running average O_3 (solid black line) and hourly average O_3 (dash-dot blue line) from the EPA
 193 surface observations at RMNP and the 3-hourly MERRA-2 reanalysis surface O_3 at the near-
 194 est grid point to RMNP (40°N , 105.625°W ; orange line) for 1 March – 30 June 2012 (time in
 195 UTC). The exceedence events where the MDA8 $O_3 \geq$ the EPA standard in 2012 (75 ppbv; dot-
 196 ted horizontal red line) are indicated by the vertical pink shading and the events that would
 197 be considered exceedences under the new EPA standard (70 ppbv; solid horizontal red line) are
 198 indicated by the vertical grey shading. The times of the SI-1 and SI-2 events, corresponding to
 199 Figs. 2-4, are indicated by the black diamonds.

241 and SI-2 events, the SI-1 is linear – stretching from Vancouver Island, Canada to the Wyoming-
 242 Colorado border – as opposed to the curved SI-2 from Washington down to Arizona and
 243 back to Montana (400 hPa, Fig. 3). Both SI events are a result of a cut-off low (COL)
 244 near the west coast of the USA in the days prior to the O_3 exceedences (not shown). Prior
 245 to the exceedence at RMNP as a result of SI-1, the tropopause fold rotates around the
 246 COL and at 500 hPa has a hooked shape off the coast of California (not shown) before
 247 becoming deformed and elongated – impacting RMNP – as the center of vorticity moves
 248 east and the western portion is being pulled west as a consequence of an Aleutian low
 249 (Fig. 3a-d). The hook shape of the SI-2 led to the longer period of high O_3 (≥ 75 ppbv)
 250 at RMNP compared to the duration of high O_3 observations associated with SI-1; as the
 251 SI-2 fold continued to rotate over the western USA at the end of May, there was con-
 252 tinued draw down of stratospheric air toward the surface over the area, unlike the SI-1
 253 event which was steered to the northeast as it decayed. It is worth noting that the tro-

SI-1



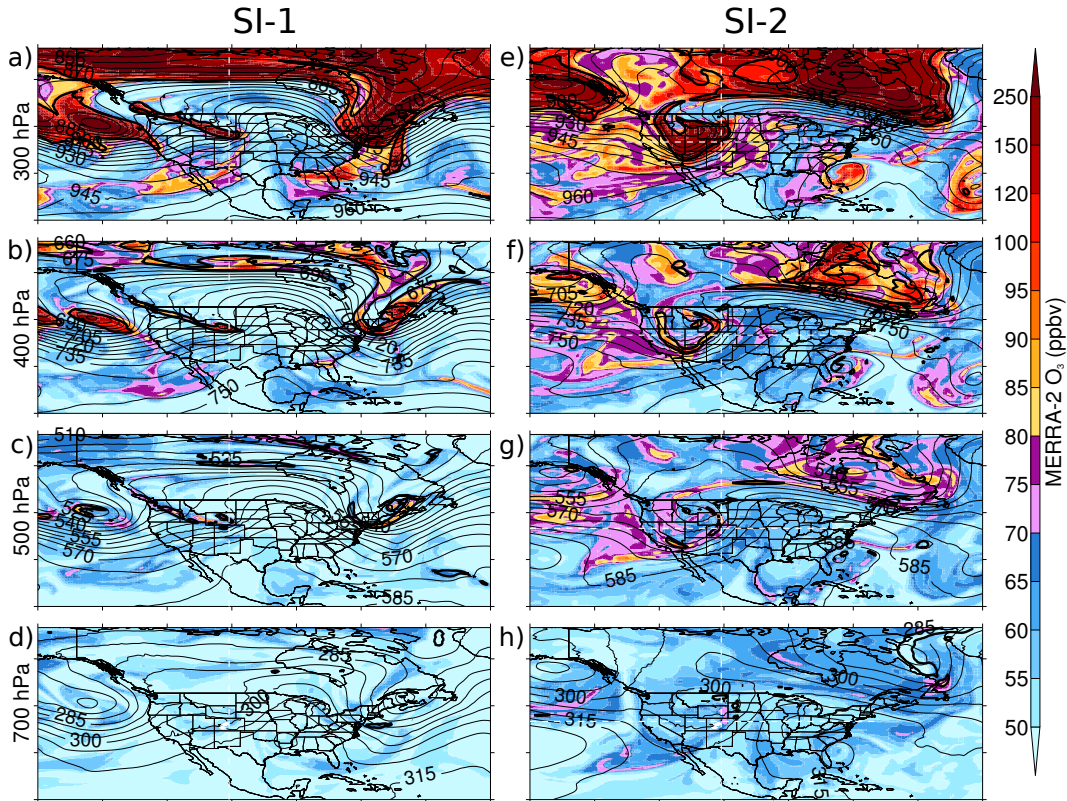
SI-2



200 **Figure 2.** (a,c) AIRS 700 hPa RH (color; %) with MERRA-2 SLP (4 hPa intervals)
 201 and (b,d) TCO from AIRS (color; Dobson unit (DU)) and MERRA-2 (dashed; 10 DU
 202 intervals) for (a,b) SI-1 and (c,d) SI-2. The approximate location of low pressure centers
 203 (“L”) and frontal boundaries – cold front (line with filled triangles (a,c)), surface
 204 trough (dashed line (a)), stationary front (filled triangles and half circles on opposite sides
 205 of line (c)), dry line (line with open half circles (c)) – are presented from the 18UTC
 206 surface analysis (close to 13:30 LT pass) on (a) March 26, 2012 and (c) May 27, 2012
 207 (www.wpc.ncep.noaa.gov/archives/web_pages/sfc/sfc_archive_maps, Accessed 8 November 2016).
 208 Note, not all fronts from the analysis archives have been depicted. The location of RMNP (pink
 209 open circle) and the Colorado state border (thick black line) are emphasized.

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pospheric background levels of MERRA-2 O₃ are qualitatively consistent with a seasonal increase in photochemical production from March (Fig. 3a-d) to May (Fig. 3e-h).



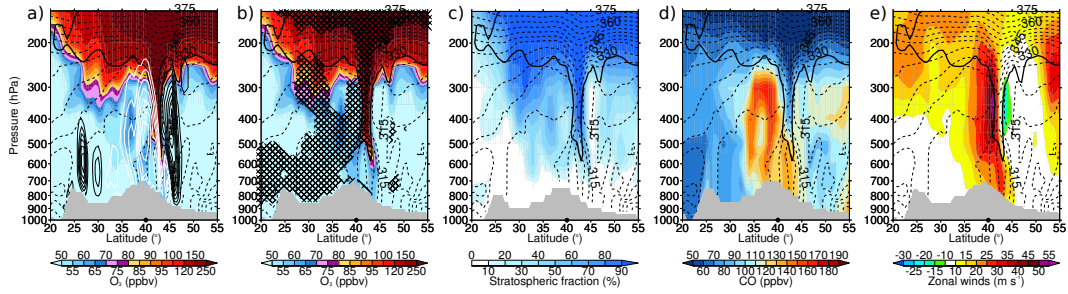
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Figure 3. O₃ distribution (color; 5 ppbv increments up to 100 ppbv and increment size increases above 100 ppbv), geopotential height (thin black contours; 5 dam intervals) and dynamical tropopause (2 PVU isosurface; thick black contour) on 300 (a,e), 400 (b,f), 500 (c,g) and 700 hPa surfaces (d,h) corresponding to the time of maximum O₃ observations at RMNP during the SI-1 event (March 27, 2012 00UTC; a-d) and the SI-2 event (May 27, 2012 09UTC; e-h). Light and dark pink color intervals highlight the previous and current EPA O₃ standard, respectively. The white dashed lines correspond to transects in Fig. 4.

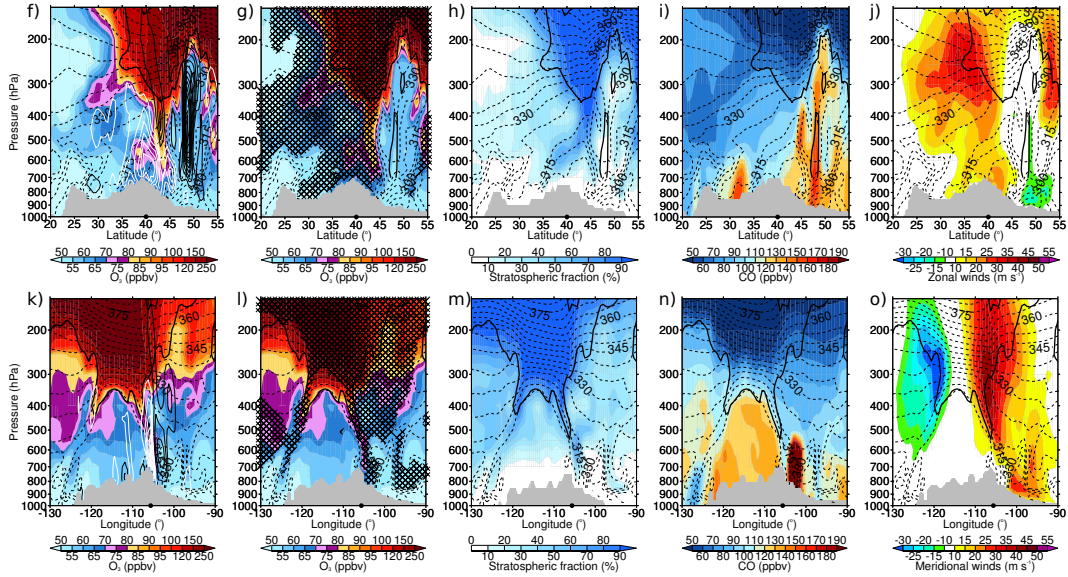
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The intrusion of air from the stratosphere into the troposphere is captured in vertical transects for the SI events in the MERRA-2 reanalysis dataset and supported by the additional GEOS-5 CO and a fraction of stratospheric air tracer (STFR) data (Fig. 4). In the N-S transect through SI-1, the dynamical tropopause and high O₃ (> 85 ppbv, Fig. 4ab; > 40% STFR, Fig. 4c) reached altitudes as low as ~600 hPa, and elevated O₃ (> 55 ppbv) reached the surface. Relatively dry air is found within the tropopause fold and in the troposphere to the south of the fold (RH < 30 %, Fig. 4b). The low CO (< 110 ppbv, Fig. 4d) reached 500 hPa within the tropopause fold; however, since the gradient in CO at the base of the fold is less than the gradient of O₃, the influence of stratospheric CO was lost due to mixing with tropospheric air characterized by higher CO mixing ratios. A strong jet at 350 hPa ($u > 50 \text{ m s}^{-1}$, Fig. 4e) connects down to the surface. There is also a clear frontal boundary on the north-side of the fold extending from an upper-level front (indicated by tight isotherms, Fig. 4a-e) down to the surface with strong descent ($\omega > 80 \text{ hPa h}^{-1}$, white contours, Fig. 4a) and strong ascent ($\omega < -80 \text{ hPa h}^{-1}$, black contours, Fig. 4a).

SI-1



SI-2



263 **Figure 4.** Vertical transects of (a-e) the SI-1 event and (f-o) the SI-2 event taken at
 264 the times of maximum O₃ observation at (a-j) 105.625°W from 20°-55°N over RMNP
 265 (black dot, 40°N) and (k-o) 40°N from 130°-90°W over RMNP (black dot, 105.625°W). O₃
 266 (a,b,f,g,k,l; ppbv), Stratospheric fraction (c,h,m; %), CO (d,i,n; ppbv), Zonal winds (e,j;
 267 m s⁻¹) and Meridional winds (o; m s⁻¹) are all shown in color with θ_e (dashed contour lines, 5 K
 268 intervals) and the isosurface of 2 PVU (thick black contour). In addition, ω (a,f,k; solid contour
 269 lines, 10 hPa h⁻¹ intervals, with white contours for descent and black contours for ascent) and
 270 RH (b,g,l; hatching < 30%) are drawn. Orography indicated by grey region.

286 Both N-S and West-East (W-E) transects are shown for the SI-2 case study (Fig. 4f-
 287 o). Although the N-S transect is shown to be just on the eastern edge of the tropopause
 288 fold (Fig. 3e-h) and the tropopause does not appear to be depressed below 350 hPa over
 289 RMNP (Fig. 4f-j), there are still strong indicators of a fold in the region. Specifically,
 290 between 35° to 45°N, there are increased levels of O₃ reaching the surface (> 65 ppbv,
 291 Fig. 4f,g) within an area marked by strong descent ($\omega > 60$ hPa h⁻¹, Fig. 4f), low hu-
 292 midity (RH < 30 % south of 45°N, Fig. 4g), large STFR (> 60 % at 600 hPa, Fig. 4h),
 293 and low CO (< 110 ppbv, Fig. 4i). The frontal boundary can be identified by the large
 294 gradients of ω and θ_e to the north of RMNP. This transect highlights the ascent ahead

295 of the front (reaching up to ~ 200 hPa at 50°N , maximum $\omega < -120$ hPa h^{-1} at 400 hPa)
296 and to a lesser extent the descent behind the front (Fig. 4f).

297 Due to the curvature of the SI-2 fold, the W-E transect intersects both sides of the
298 hook as seen at 400 hPa in Fig. 3f. The W-E transect captures the tropopause fold at
299 105°W over RMNP reaching 550 hPa as well as the western portion of the fold reach-
300 ing below 400 hPa at 120°W (Fig. 4k-o). Figure 4o shows the strong jet on both sides
301 of the curved tropopause fold ($v > 40$ m s^{-1} at 105°W and $v < -30$ m s^{-1} at 120°W).
302 The front above RMNP is also seen in this transect by the large gradients in both ω (Fig. 4k)
303 and θ_e (Fig. 4k-o). Specifically, isentropic descent above RMNP brings dry, O_3 -rich air
304 from the stratosphere towards the surface ($\text{O}_3 > 80$ ppbv and STFR $> 70\%$ at 600 hPa,
305 $\text{O}_3 > 65$ ppbv at surface, Fig. 4k-m). It is interesting to note that low CO (< 110 ppbv,
306 Fig. 4n) is simulated to reach the surface at RMNP, despite the large CO values to the
307 east emitted by a nearby fire. Biomass burning emissions used in the GEOS-5 simula-
308 tion of CO follow the Quick Fire Emission Dataset (QFED) version 2.4r6 which is based
309 on MODIS satellite fire radiative power (FRP) [Darmenov and da Silva, 2015].

310 4 Conclusions

311 Stratospheric intrusions have been the interest of decades of research, especially
312 for the potential influence on ground-level O_3 concentrations. However, until recently,
313 the fine-scale nature of the O_3 filaments have been misrepresented in models and reanal-
314 yses, as the features of an SI are best identified in horizontal resolutions of 50 km or smaller
315 [Büker et al., 2005; Lin et al., 2012; Ott et al., 2016]. For this reason, and likely because
316 reanalysis O_3 corresponds better with independent observations in the stratosphere than
317 in the troposphere [Dragani, 2011; Wargan et al., 2015, 2017], there are very few stud-
318 ies of stratosphere-to-troposphere transport which use reanalysis O_3 [Škerlak et al., 2014;
319 Zanis et al., 2014; Knowland et al., 2015, 2017; Ott et al., 2016; Ryoo et al., 2017]. NASA’s
320 MERRA-2 reanalysis is such a high-resolution dataset, which benefits from assimilated
321 O_3 to present O_3 on the same spatiotemporal resolution as the meteorology. Here, two
322 case study examples of SI events which were known to impact surface O_3 air quality are
323 examined. The SI events are diagnosed by the folding of the tropopause under the jet
324 stream and subsequent isentropic descent of dry, O_3 -rich/ CO -poor stratospheric air to-
325 wards the surface using the MERRA-2 reanalysis in combination with surface O_3 and
326 satellite observations and GEOS-5 simulated CO and a stratospheric tracer. We show
327 that MERRA-2, a publicly-available dataset, can be used in scientific studies to iden-
328 tify SIs by both atmospheric dynamics and composition. This is a proof of concept study
329 opening the door to detailed multi-year analyses of stratospheric intrusions over the USA
330 and worldwide. Though the MERRA-2 reanalysis tends to underestimate the magnitude
331 of surface O_3 during the SIs [see also Ott et al., 2016], the combination of meteorolog-
332 ical variables and O_3 for a relatively long period of time to within a few weeks of present
333 time may provide a valuable and unique tool for air quality managers [Kaldunski et al.,
334 2017] and scientific studies of stratospheric intrusions.

335 It is important to be able to identify the differences in anthropogenic and natural
336 sources of O_3 , especially on exceedence days. Since the GEOS-5 model used to produce
337 MERRA-2 does not simulate full O_3 chemistry in the troposphere, we are unable to de-
338 termine the influence of stratospheric O_3 on surface concentrations separate from photochemically-
339 produced O_3 , especially in late spring/early summer. The impact of photochemically-
340 produced O_3 on total O_3 later in the spring will be explored in more detail using the GEOS-5
341 chemistry climate model in a future publication. Yet this study presents strong evidence
342 that the MERRA-2 reanalysis can be used in the identification of SIs.

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348 satellite data (AIRX3STD_V006) are available through the NASA GES DISC online archive
349 (<https://disc.gsfc.nasa.gov/>). Tables of the hourly and 8-hourly average O₃ observations
350 are available to download on the EPA’s website ([http://aqsd1.epa.gov/aqsweb/aqstmp/airdata/
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