



Evaluating a fire smoke simulation algorithm in the National Air Quality Forecast Capability (NAQFC) by using multiple observation data sets during the Southeast Nexus (SENEX) field campaign

Li Pan^{1,2}, Hyun Cheol Kim^{1,2}, Pius Lee¹, Rick Saylor³, YouHua Tang^{1,2}, Daniel Tong^{1,2}, Barry Baker^{1,2}, Shobha Kondragunta⁴, Chuanyu Xu⁵, Mark G. Ruminski⁴, Weiwei Chen^{1,6}, Jeff Mcqueen⁷ and Ivanka Stajner⁸

¹ NOAA/OAR/Air Resources Laboratory, College Park, MD 20740, USA

² UMD/Cooperative Institute for Climate and Satellites, College Park, MD 20740, USA

³ NOAA/OAR/ARL/Atmospheric Turbulence and Diffusion Division, Oak Ridge, TN 37830, USA

⁴ NOAA/NESDIS, College Park, MD 20740, USA

⁵ I. M. Systems Group at NOAA, College Park, MD 20740, USA

⁶ Northeast Institutes of Geography and Agroecology, Chinese Academy of Sciences, Changchun 130102, P. R. China

⁷ NOAA/NCEP/Environmental Modeling Center, College Park, MD 20740, USA

⁸ NOAA/NWS Office of Science and Technology Integration, Silver Spring, MD 20910, USA

Correspondence to: Li.Pan@noaa.gov



25 Abstract

26 Multiple observation data sets: Interagency Monitoring of Protected Visual Environments
27 (IMPROVE) network data, Automated Smoke Detection and Tracking Algorithm (ASDTA), Hazard
28 Mapping System (HMS) smoke plume shapefiles and aircraft acetonitrile (CH_3CN) measurements from
29 the NOAA Southeast Nexus (SENEX) field campaign are used to evaluate the HMS-BlueSky-SMOKE-
30 CMAQ fire emissions and smoke plume prediction system. A similar configuration is used in the US
31 National Air Quality Forecasting Capability (NAQFC). The system was found to capture most of the
32 observed fire signals. Usage of HMS-detected fire hotspots and smoke plume information were valuable
33 for both deriving fire emissions and forecast evaluation. This study also helped identified that the
34 operational NAQFC did not include fire contributions through lateral boundary conditions resulting in
35 significant simulation uncertainties. In this study we focused both on system evaluation and evaluation
36 methods. We discussed how to use observational data correctly to filter out fire signals and
37 synergistically use multiple data sets. We also addressed the limitations of each of the observation data
38 sets and evaluation methods.

39 Introduction

40 Wildfires and agricultural/prescribed burns are common in North America all year round, but
41 predominantly occur during the spring and summer months (Wiedinmyer et al., 2006). These fires pose
42 a significant risk to air quality and human health (Delfino et al., 2009; Rappold et al., 2011; Dreessen et
43 al., 2016; Wotawa and Trainer 2000; Sapkota et al., 2005; Jaffe et al., 2013; Johnston et al., 2012). Since
44 January 2015, smoke emissions from fires have been included in the National Air Quality Forecasting
45 Capability (NAQFC) daily $\text{PM}_{2.5}$ operational forecast (Lee et al., 2017). The NAQFC fire simulation consists
46 of: the NOAA National Environmental and Satellite Data and Information Service (NESDIS) Hazard
47 Mapping System (HMS) fire detection algorithm, the U.S. Forest Service (USFS) BlueSky-fire emissions



estimation algorithm, the U.S. EPA Sparse Matrix operator Kernel Emission (SMOKE) applied for fire plume rise calculations, the NOAA National Weather Service (NWS) North American Multi-scale Model (NAM) for meteorological prediction and the U.S. EPA Community Multi-scale Air Quality Model (CMAQ) for chemical transport and transformation. In contrast to most anthropogenic emissions, smoke emissions from fires are largely uncontrolled, transient and unpredictable. Consequently, it is a challenge for air quality forecasting systems such as NAQFC to describe fire emissions and their impact on air quality (Pavlovic et al., 2016; Lee et al., 2017; Huang et al., 2017).

Southeast Nexus (SENEX) was a NOAA field study conducted in the Southeast U.S. in June and July 2013 (Warneke et al., 2016). This field experiment investigated the interactions between natural and anthropogenic emissions and their impact on air quality and climate change (Xu et al., 2016; Neuman et al., 2016). In this work, we used the SENEX dataset to evaluate the HMS-BlueSky-SMOKE-CMAQ fire simulations during the campaign period.

Two simulations were performed: one with and one without smoke emissions from fires during the SENEX field campaign. Due to the large uncertainties in the estimates of fire emissions and smoke simulations (Baker et al., 2016; Davis et al., 2015; Drury et al., 2014), the first step of the evaluation focused on the fire signal capturing capability of the system. Differences between the two simulations represented the impact of the smoke emissions from fires on the CMAQ model results. Observations from various sources were utilized in this analysis: (i) ground observations (Interagency Monitoring of Protected Visual Environments (IMPROVE)), (ii) satellite retrievals (Automated Smoke Detection and Tracking Algorithm (ASDTA) and HMS smoke plume shape), and (iii) aircraft measurements (SENEX campaign). Fire signals predicted by the modeling system were directly compared to these observations. Several criteria have been used to rank efficacy of the observation systems for fire induced pollution plumes.



71 **Methodology**

72 In this section we introduce the NAQFC fire modeling system used in the study. Uncertainties
73 and limitations in the various modeling components of the system are discussed. Fig. 1 illustrates the
74 schematics of the system. There are four processing steps:

75 **HMS (Hazard Mapping System)**

76 The NOAA NESDIS HMS is a fire smoke detection system based on satellite retrievals. The
77 satellite constellation used comprised of 2 Geostationary Operational Environmental Satellite (GOES-10
78 and GOES-12) and 5 polar orbiting satellites (MODIS (Moderate-resolution Imaging Spectroradiometer))
79 -- Terra and Aqua, AVHRR (Advanced Very High Resolution Radiometer) 15/17/18). HMS detects
80 wildland fire locations and analyzes their sizes, starting times and durations (Ruminski et al., 2008;
81 Schroeder et al., 2008; Ruminski and Kondragunta 2006).

82 HMS first processes satellite data by using automated algorithms for each of satellite platforms
83 to detect fire locations (Justice et al., 2002; Giglio et al., 2003; Prins and Menzel 1992; Li et al., 2000),
84 which is then manually analyzed by analysts to eliminate false detections and/or add missed fire
85 hotspots. The size of the fire is represented by the number of detecting pixels corresponding to the
86 nominal resolution of MODIS or AVHRR data. Fire starting times and durations are estimated from close
87 inspection of the visible band satellite imagery. A bookkeeping file is generated at the end of this
88 detection step, named "hms.txt". It includes all the thermal signal hotspots detected by the
89 aforementioned 7 satellites. During the analyst quality control step, detected potential fire hotspots
90 lacking visible smoke in the retrieval's RGB real-color imagery are removed resulting in a reduced fire
91 hotspot file called either "hmshysplit.prelim.txt" or "hmshysplit.txt" to be input into the BlueSky
92 processing step.



In general, “hmsysplit.prelim.txt” and “hmsysplit.txt” are very similar, and “hmsysplit.txt” is created later than “hmsysplit.prelim.txt” (Fig. 1). But the differences between “hmx.txt” and “hmsysplit.txt” (“hmsysplit.prelim.txt”) can be rather substantial. The reasons for differences are: 1) many detected fires do not produce detectable smoke; 2) some fires/hotspots are detected only at night, when smoke detection is not possible; 3) smoke emission RGB imageries are obscured by clouds thus not detected by the analyst. Therefore, smoke emission occurrence provided by the HMS is a conservative estimate of fire emissions.

By using multiple satellites the likelihood of detecting fires in HMS is robust. However, when the fire geographical size is small the HMS detection accuracy dramatically decreases (Zhang et al., 2011; Hu et al., 2016). Other limitations of the HMS fire detections include ineffective retrievals at nighttime and under cloud cover.

BlueSky

BlueSky, developed by the USFS (US Forest Service), is a modeling framework to simulate smoke impacts on regional air quality (Larkin et al., 2009; Strand et al., 2012). In this study, BlueSky acted as a fire emission model to provide input for SMOKE (Herron-Thorpe et al., 2014; Baker et al., 2016). BlueSky calculates fire emission based on HMS-derived locations (Fig. 1).

Fire geographical extent is reflected by the number of nearby fire pixels detected by satellites in a 12 km resolution CMAQ model grid. Fire pixels are converted to fire burning areas in BlueSky based on the assumption that each fire pixel has a size of 1 km² and 10% of its area can be considered as burn-active (Rolph et al., 2009). All fire pixels in a 12 km grid square are aggregated. BlueSky uses the following to estimate biomass availability: fuel loading map is from the US National Fire Danger Rating System (NFDRS) for the Conterminous US (CONUS) with the exception in western US where the HARDY set is used (Hardy and Hardy 2007). BlueSky uses Emissions Production Model (EPM) (Sandberg and



Peterson 1984), a simple version of CONSUME, to calculate fuel actually burned -- the so-called consumption sums. Finally, EPM is also used in BlueSky to calculate the fire emission hourly rate per grid-cell. BlueSky outputs CO, CO₂, CH₄, non-methane hydrocarbons (NMHC), total PM, PM_{2.5}, PM₁₀ and heat flux (Fig. 1).

BlueSky does not iteratively recalculate fire duration according to the modeled diminishing fuel loading or the modeled fire behavior. In the aggregation process, when there is more than one HMS point in a grid cell which have different durations, all points in that grid cell would be assigned the largest duration in all points. For an example, if there were 3 HMS points that had durations of 10, 10 and 24 hours, the aggregation would include 3 points (representing 3 km²) assigned with 24 hour duration to all of the 3 HMS points.

HMS has no information about fuel loading. BlueSky uses a default fuel loading climatology over the eastern US. BlueSky uses an idealized diurnal profile for fire emissions. Uncertainties in fire sizes, fuel loading and fire emissions rate lead to large uncertainties in wildland smoke emissions (Knorr et al., 2012; Drury et al., 2014; Davis et al., 2015).

SMOKE

In SMOKE (Sparse Matrix Operator Kernel Emission), the BlueSky fire emissions data in a longitude-latitude map projection are converted to CMAQ ready emission gridded files (Fig. 1). Fire smoke plume rise is calculated using formulas by Briggs. The heat flux from BlueSky and NAM meteorological state variables are used as input (Erbrink 1994). The Briggs' algorithm calculates plume top and plume bottom, between plume top and bottom the emission fraction is calculated layer by layer assuming a linear distribution of flux strength in atmospheric pressure. For model layers below the plume bottom the emission fraction is assumed to be entirely in the smoldering condition as a function of the fire burning area.



We adopted a speciation cross-reference map to match BlueSky chemical species to that in CMAQ using the U.S. EPA Source Classification Codes (SCCs) for forest Wildfires (<https://ofmpub.epa.gov/scsearch/docs/SCC-IntroToSCCs.pdf>). The life-span of fire is based on the HMS detected fire starting time and duration. During fire burning hours a constant emission rate is assumed. This constant burn-rate has been shown to be a crude estimate (Saide et al., 2015; Alvarado et al., 2015). Other uncertainties include plume rise (Sofiev et al., 2012; Urbanski et al., 2014; Achtemeier et al., 2011) and fire-weather (fire influencing local weather).

CMAQ

The CMAQ version 4.7.1 was used. We chose the CB05 gas phase chemical mechanism (Yarwood et al., 2005) and the AERO5 aerosol module (Carlton et al., 2010). Anthropogenic emissions were based on the U.S. EPA 2005 National Emission Inventory (NEI) projected to 2013 (Pan et al., 2014), Biogenic emissions (BEIS 3.14) were calculated in-line inside CMAQ.

Simulations

The NAM provided meteorology fields to drive CMAQ (Chai et al., 2013). NAM meteorology is evaluated daily and results (BIAS and RMSE etc.) are posted on: “<http://www.emc.ncep.noaa.gov/mmb/mmbpll/mmbverif/>”. The simulation domain is shown in Fig. 1. It includes two domains: (i) a 12km domain covering the Continental U.S. (CONUS); and (ii) a 4km domain covering the Southeast U. S. where the majority of SENEX measurements occurred. Lateral boundary conditions (LBC) used in the smaller SENEX domain simulation were extracted from that from the CONUS simulations. Four scenarios were simulated: CONUS with fire emissions, CONUS without fire emissions, SENEX with fire emissions and SENEX without fire emissions.

There were several differences in system configuration between the NAQFC fire smoke forecasting and the “with-fire” simulation in this study. For models, the BlueSky versions used in NAQFC



162 and that in this study are v3.5.1 and v2.5, respectively; CMAQ versions used in NAQFC and in this study
163 are v5.0.2 and v4.7.1, respectively. For simulations, current fire smoke forecasting in the NAQFC
164 includes two runs: the analysis and the forecast (Huang et al. 2018 (manuscript in preparation)). The
165 analysis run is a 24-hour retrospective simulation to rerun yesterday's fire emissions using yesterday's
166 meteorology providing an initial condition for today's forecast. The forecast run is a 48-hour forecasting
167 simulation to run yesterday's fire emissions to be projected as continued fires had their burn duration
168 were more than 24 hours. The "with-fire" simulation in this study is exactly identical to the analysis run
169 in NAQFC.

170 Evaluations

171 Carbon monoxide (CO) has a relatively long life time in the air and is commonly associated with
172 biomass burning. CO was used as a fire tracer in the prediction. The CO difference (ΔCO) between
173 CMAQ simulations with and without fire emissions was used as the indicator of fire influence. For
174 additional observations we used: potassium (K) collected at the IMPROVE (Interagency Monitoring of
175 Protected Visual Environments) sites within the SENEX domain; acetonitrile (CH_3CN) measured from the
176 SENEX campaign flights; and fire plume shape detected by the HMS analysis as real fire signals. The
177 enhancement in ΔCO concentration due to fire was directly compared with those signals. At the same
178 time, ΔAOD (Aerosol Optical Depth) from CMAQ ("with-fire" simulated concentration minus that with
179 "without-fire") was also used as fire indicator when compared with smoke masks given by the ASDTA
180 (Automated Smoke Detection and Tracking Algorithm).

181 In this study, we have focused on evaluations subject to the large uncertainties of the underlying
182 physical processes of smoke emissions from fires and its transport. In each modeling step in HMS,
183 BlueSky, SMOKE and CMAQ, the modeling system accrues uncertainties. Such uncertainties were likely
184 cumulative and might lead to larger error in succeeding components (Wiedinmyer et al., 2011). For an



185 example, heat flux from BlueSky influenced plume rise height in SMOKE and consequently influenced
186 plume transport in CMAQ. It is also noteworthy that when we compared modeled ΔCO against
187 measured K or CH_3CN , the objective was to search for enhancement signals resulting from fires but it
188 was not aiming to account for proportional concentration changes in the tracers. Attempting to account
189 for CMAQ simulation uncertainties in surface ozone and particulate matter as a function of smoke
190 emissions from fires was difficult. Neither was it the objective of this study. Rather, the purpose of this
191 study is to focus on analyzing the capability of the HMS-BlueSky-SMOKE-CMAQ modeling system to
192 capture the timing of fire signals.

193 The SENEX campaign occurred in June and July and our model simulations were from June 10 to
194 July 20, 2013. Throughout the campaign we used all available observation datasets including ground-,
195 air- and satellite-based acquired data. Each dataset had its unique characteristics and linking them
196 together gave an overall evaluation. At the same time, in each dataset our evaluations included as many
197 as possible observed fire cases. Both well-predicted and poorly-predicted cases are presented to
198 illustrate potential reasons responsible for the modeling system's behavior.

199 **Results and Discussions**

200 **Observed CO versus modeled CO in SENEX**

201 Table 1 lists observed and modeled CO vertical profiles for the “with-fire” and “without-fire”
202 cases during the SENEX campaign. Observed CO concentrations between the surface and 7 km AGL
203 (Altitude above Ground Level) in the SENEX domain area remained greater than 100 ppb during all 40
204 days of the campaign. The highest CO concentrations were measured closer to the surface. The
205 maximum measured CO concentration of 1277 ppb was observed during a flight on July 03 at an ASL
206 (Altitude above Sea Level) of 974 m. In this flight strong fire signals were observed but the fire
207 simulation system missed those signals as discussed below.



CO concentrations were underestimated by the model in almost all cases even when the model captured CO contribution from fire emissions spatio-temporarily. Mean ΔCO in each height interval was usually above 1.5 ppb but less than 2.0 ppb. Fig. 2a exhibits the contribution of total CO emissions from fires which occurred inside the SENEX domain over the simulation period. The maximum CO emissions contribution from fires was about 3% during the campaign. In most of those days fire emission contributions in SENEX were less than 1%. The averaged contribution during those 40 days was 0.7%. Fig. 2b exhibits the contribution of CO flowing into the SENEX domain from its boundary caused by fire outside the SENEX domain but inside the CONUS domain (Fig. 1). The averaged fire contribution to CO from outside the SENEX domain was 0.67%. CO influenced by fire emission in June is greater than that in July.

During the field experiment the general lack of large fires made evaluation of modeled fire signature difficult since it was easier to capture large fire signals than the smaller fires. We postulated that a clear fire signal simulated in the HMS-BlueSky-SMOKE-CMAQ system could be indicated by ΔCO significantly larger than its temporal averages resulted by fires originated from inside and/or outside the SENEX domain. For an example, if a clear fire signal between 500 m and 1000 m AGL is represented by ΔCO in a model simulation and the concentration of ΔCO is above 2.0 ppb, based on the average CO concentration of about 150 ppb as well as on with SENEX domain and outside of SENEX domain fire contributions of $(150 \times (0.007 + 0.0067)) = 2.0$.

Figure 3 displays the simulated ΔCO extracted along a SENEX flight path. The modeled concentration showed that the fire impacts on SENEX were not negligible perspective despite a lack of larger fire events as shown in Fig. 2a and 2b during the SENEX campaign period. That confirmed the importance of evaluating the fire simulation system in an air quality model. Unless a model is able to predict fire signals correctly it is useless for modelers to discuss fire effects on chemical composition of



the atmosphere. A detail of how our model caught or missed or falsely predicted fire signals during the SENEX campaign and a comparison of ΔCO versus CH_3CN will be discussed in the follow discussion.

IMPROVE

The Interagency Monitoring of Protected Visual Environments (IMPROVE) is a long term air visibility monitoring program initiated in 1985 (<http://vista.cira.colostate.edu/Improve/data-page>). It provides 24-h integrated particulate matter (PM) speciation measurements every third day (Malm et al., 2004; Eatough et al., 1996). The IMPROVE dataset was chosen for this analysis because it included K (potassium), OC (organic carbon) and EC (elemental carbon), important fire tracers. IMPROVE monitors are ground observation sites likely influenced by nearby fire sources.

There were 14 IMPROVE sites in the SENEX domain (Fig. 4). Potential fire signals were identified by using CMAQ modeled ΔCO and IMPROVE observed K. However, in addition to fires K has multiple sources such as soil, sea salt and industry. Co-incidentally fires should also produce enhanced EC and OC concentrations, a fire signal should reflect above-average values for EC, OC, and K. EC, OC and K observations that were 20% above their temporal averages during the SENEX campaign were used as a predictor for fire event identification. Meanwhile, co-measured NO_3^- and SO_4^{2-} concentrations 50% below their respective temporal averages was used to screen out data with industrial influences. Lastly, a third predictor was employed so that concentrations of other soil components besides K should be below their temporal average to eliminate conditions of spikes in K concentration due to dust. With these three criteria the IMPROVE data was screened for fire events (See Table 2).

Five fire events were observed at four IMPROVE sites. Table 2 lists measured EC, OC, NO_3^- , K, soil and SO_4^{2-} concentrations ($\mu\text{g m}^{-3}$) and their ratios to averages. BC versus OC and K versus BC ratios were also calculated and listed in Tab. 2 to illustrate the application of our criteria. We found that except for monitor BRIS, all other sites (COHU, MACA and GRSM) had BC/OC and K/BC ratios comparable to the



254 ratios of the same quantities due to biomass burning reported by other researchers (Reid et al., 2005;
255 DeBell et al., 2004). BRIS is a coastal site likely influenced by sea salts (Fig. 4).

256 For the four identified fire cases, we plotted ΔCO as a modeled fire tracer around the IMPROVE
257 sites. Our model simulation reproduced fire signals on June 21 at COHU and GRSM and on June 24 at
258 MACA. We used the June 24 MACA case as an example (see Fig. 4) -- closed black circles represent the
259 detected fire locations; closed triangles represents IMPROVE sites, and ΔCO values above 2.0 ppb were
260 shown. On June 24, 2013, detected fire spots were outside the SENEX domain, but SSW wind blew
261 smoke plumes into the SENEX domain and affected modeled CO in MACA. Modeled ΔCO in MACA was 5
262 ppb.

263 Another IMPROVE site located upwind of MACA, CADI, was also potentially under the influence
264 of that fire event; however, data from CADI on June 24 did not indicate a fire influence, possibly due to
265 the frequency of IMPROVE sampling that eluded measurement or that the smoke plume was
266 transported above the surface in disagreement with what was modeled. Within the four fire cases
267 identified by the IMPROVE data during SENEX (Tab. 2), the model successfully captured three out of four
268 events. The model missed fire signal on July 3 at MACA. The model missed the fire signal on July 3 at
269 MACA. The following section is dedicated for the July 3 SENEX flight.

270 **Plume Spatial Coverage**

271 HMS determines fire hotspot locations associated with smoke and upon incorporating the
272 smoke plume shape information from visible satellite images. HMS provides smoke plume shapefiles
273 over much of North America. We focused on the shapefile over CONUS – a two-dimensional smoke
274 plume spatial depiction collapsing all plume stratifications to a satellite eye-view. For modeled plumes,
275 we integrated modeled ΔCO by multiplying the layer values with the corresponding CMAQ model layer



276 thicknesses and air density to derive a simulated smoke plume shape. HMS-derived smoke plume shape
277 versus CMAQ predicted smoke plume shape was then used to evaluate the fire simulation.

278 Figure of Merits in Space (FMS) (Rolph et al., 2009) is a statistic for spatial analysis and was
279 calculated as follows:

$$FMS = \frac{Area_{hms} \cap Area_{cmaq}}{Area_{hms} \cup Area_{cmaq}} \times 100\%$$

280 Where Area_hms represents area of grid cells influenced by fire emission over CONUS detected by HMS
281 and Area_cmaq represents area of grid cells over CONUS identified by model prediction. In general, a
282 higher FMS value indicates a better agreement between the observed and modeled plume shape (Rolph
283 et al., 2009).

284 Figure 5 summarizes FMS during the SENEX campaign. Average FMS was 22% with its maximum
285 at 56% on July 6 and minimum at 1.2% on June 17 2013. Figure 6a exhibits HMS detected smoke plume
286 and CMAQ calculated smoke plume over CONUS on July 6. The light blue shading represents modeled
287 plume shape (defined as total column ΔCO) and the thin dash line and emboldened green lines encircle
288 areas representing HMS-derived light and strong influenced plume shape, respectively (Fig. 6a). The FMS
289 score was 56% meaning that the modeled plume shape was consistent with that of HMS. However,
290 CMAQ might have underestimated the intensive fire influence areas along the border of California and
291 Nevada. Subsequently, the model also under-predicted its associated influence in North Dakota, South
292 Dakota, Minnesota, Iowa and Wisconsin.

293 Figure 6b exhibits the worst case on June 17 2013 in terms of resulting with a FMS score at 1.2%.
294 Two reasons led to this: (i) CMAQ missed fire emissions from Canada. Those fire sources located outside
295 the CONUS modeling domain and our simulation system used a climatologically-based static LBC;
296 Secondly on June 17, there were a lot of fire hotspots in the Southeastern U.S., i.e., in Louisiana,



297 Arkansas and Mississippi along the Mississippi River. Hotspots were detected but they lacked associated
298 smoke in corresponding RGB imagery (Fig. 6c). This could be due to cloud blockage or to small
299 agricultural debris clearing, burns in under-bushes or prescribed burns. These conditions prevented the
300 HMS from identifying fires and hence emissions were not modeled for those sources.

301 It is noteworthy that the FMS evaluation contained uncertainties contributed from both
302 modeled and observed values. The calculated campaign duration and SENEX-wide averaged FMS was
303 22%. It is significantly higher than that achieved by a similar analyses done by HYSPLIT (Hybrid Single
304 Particle Lagrangian Integrated Trajectory) smoke forecasting for the fire season of 2007 (6.1% to 11.6%)
305 (Rolph et al., 2009). The primary reason is that the HYSPLIT smoke simulation accessed at the invocation
306 of a forecast cycle the HMS fire information which is already one day old due to retrieval latency and
307 cycle-queuing issues. However, our model simulation in this study was from a retrospective module
308 using current day HMS fire information. Such discrepancies have been discussed by Huang et al. 2018
309 (*manuscript in preparation*). Other reasons, such as plume rise, etc. were discussed in the following
310 section on ASDTA.

311 **ASDTA**

312 The Automated Smoke Detection and Tracking Algorithm (ASDTA) is a combination of two data
313 sets: (1) the NOAA Geostationary satellite (G13) retrieves aerosol optical depth using visible channels
314 and produces a product called GOES Aerosol/Smoke Product (GASP) (Prados et al., 2007); and, (2) the
315 NOAA HYSPLIT dispersion model predicts smoke plume direction and extension (Draxler and Hess 1998).
316 ASDTA provides the capability to determine whether the GASP is influenced by one or multiple smoke
317 plumes over a location at a certain time. The ASDTA is a signature identification analysis. On the other
318 hand, the HYSPLIT smoke forecast is based on the HMS fire detection and BlueSky emission modeling
319 driven by the NOAA NWS regional meteorology model. These data are suitable for model performance



320 evaluation in this study. For each simulation, modeled AOD was calculated for each sensitivity test
 321 (“with-fire” or “without-fire”) and ΔAOD is defined as the difference obtained by subtracting
 322 $\text{AOD}_{\text{without-fire}}$ from $\text{AOD}_{\text{with-fire}}$.

323 Figure 7a illustrates a GOES retrieved AOD (summed over from 10:00 am to 2:00 pm at local
 324 time) contour plot that reflects influences by smoke plumes over the CONUS domain on June 14 2013.
 325 Color-shaded region represents the fire-smoke influenced areas and the color denotes the magnitude of
 326 the retrieved AOD (Fig. 7a). Figure 7b presents similar results, but for simulated ΔAOD (with-fire –
 327 without-fire). For further evaluation of the HMS detected smoke plume shape Fig. 7c can be compared
 328 with Figs. 7a and 7b.

329 Figure 7a shows several regions under the influence of fires in: California, northwest Mexico,
 330 Kansas, Missouri, Oklahoma, Arkansas, Texas and part of the Gulf of Mexico. In the northeastern USA,
 331 fire plumes occurred sparingly. Those regions agreed relatively well with the shaded contours between
 332 Figs. 7a and 7c. However, due to the lack of fire treatments in the CMAQ LBC, the simulation (Fig. 7b)
 333 missed smoke influence on the northeast region of the CONUS domain. CMAQ also failed to simulate
 334 the fire influences in the southwest region of the domain.

335 Similar plots for June 25 are shown in Figs. 7d, 7e and 7f for ASDTA, CMAQ and HMS,
 336 respectively. The ASDTA (Fig. 7d) predicted an overestimation in fire influences in the south including
 337 Texas and the Gulf of Mexico and an underestimation in the northeastern U.S. On the other hand, the
 338 model predicted two strong fire signals clearly: near the border between Arizona and Mexico, and in
 339 Colorado (See Fig. 7e). All the fire influenced areas in Fig. 7e were seen in Fig. 7f --- reflecting
 340 observation by HMS.

341 Comparing ASDTA plots and CMAQ ΔAOD plots (Fig. 7a vs 7b; Fig. 7d vs 7e), we found both
 342 similarities and differences. Similarities were attributable to similar fire accounting, smoke emissions



from fires calculation and meteorology. Differences were attributable to: (i) HYSPLIT smoke simulation used more fire hotspots than that used by CMAQ due to domain size; (ii) only fires inside the CONUS were included in the CMAQ fire simulation and LBCs did not vary to reproduce impacts of wildfires from outside of the domain; (iii) Despite both the HYSPLIT and CMAQ fire plume rise were estimated by the Briggs' equation, the HYSPLIT plume rise was limited to 75% of the mixed layer height (MLH) at daytime and two times MLH at nighttime, whereas the CMAQ fire plume rise did not have these limitations.

SENEX

SENEX (Southeast Nexus) was a field campaign conducted by NOAA in cooperation with the US EPA and the National Science Foundation in June and July 2013. Although SENEX was not specifically designed for fire studies, its airborne measurements included $PM_{2.5}$ OC and EC, CO and acetonitrile (CH_3CN). CH_3CN was chosen as a fire tracer since it is predominantly emitted from biomass burning (Holzinger et al., 1999; Singh et al., 2012).

CH_3CN has a residence time in the atmosphere of around 6 months (Hamm and Warneck 1990) and the reported CH_3CN background concentration is around 100 - 200 ppt (Singh et al., 2003). Measured CH_3CN concentrations tend to increase with altitude (Singh et al., 2003; de Gouw et al., 2003), since biomass burning plumes are subject to ascend during long-range transport. During SENEX, measured CH_3CN showed a similar pattern. Fire signals were identified through airborne measurements of CH_3CN when its concentration exceeded the background; e.g., on July 3 2013, or when its concentration peak appeared at high altitude; e.g., on June 16 2013 and July 10 2013.

CH_3CN airborne measurements were used to identify fire plumes at certain locations and heights during SENEX. For model evaluations, fire locations and accurate meteorological wind field are crucial to interpret 2-D measurements such as IMPROVE, HMS and ASDTA. To verify a 3-D fire field, it is critical to capture plume rise. However, it was extremely difficult to back out plume rise from the



airborne measurements. An additional uncertainty arose in the difference of temporal resolutions of the data: IMPROVE, HMS shapefiles and ASDTA were daily or hourly data, whereas airborne CH_3CN data were measured at one-minute intervals.

Figure 8a shows a CMAQ simulated ΔCO vertical distribution along flight transects on June 16 2013. The x-axis label is UTC (hour) and the y-axis label is AGL (m). Two color bars represent observed CH_3CN concentration (rectangle bar in ppt) and simulated ΔCO concentration (fan bar in ppb), respectively. This flight occurred during the weekend over and around power plants around Atlanta, GA. The color of flight path represents observed CH_3CN concentration in ppt. In Fig. 8a, the concentration of ΔCO increased from surface to 5000 m, especially above 2000 m. Six CH_3CN concentration peaks were observed when AGL was above 2500 m.

For CMAQ simulated ΔCO , five out of six fire signals detected by CH_3CN measured spikes were captured where ΔCO concentrations were all above 3 ppb. Only one fire signal was missed by the model at 18:30 UTC June 16 2013. Model simulation showed that long range transports (LRT) of smoke plumes influenced airborne observations. Fire signals from the free troposphere subsided and influenced flight measurements. High EC or OC or CO did not concur with high CH_3CN observation probably due to species lifetime differences. HMS smoke plume did not show any hotspots or smoke plume around Atlanta suggesting that the sources of those observed fire signals were not from its vicinity.

A similar phenomenon was seen in SENEX flight 0710, which occurred during flight transects from Tennessee to Tampa, FL. Figure 8b is a similar graph as Fig. 8a. Based on ΔCO concentrations, CMAQ captured the July 10 case as fire signals were observed. Nonetheless, ΔCO may be over predicted at around 19 UTC. The model exhibited a fire signal with ΔCO concentration of about 3 ppb near 6000 m around 19 UTC, whereas measured CH_3CN was 120 ppt and decreased with AGL.



388 **SENEX flight on July 3**

389 Observations from IMPROVE, HMS and SENEX identified fire signals on July 3 2013. ASDTA
390 retrievals were not available. Those signals were missed by the model. In this section, we will use all of
391 evaluation methods addressed above to study potential causes of failure of the model to reproduce fire
392 signals.

393 At the MACA IMPROVE site on July 3 2013, the wind direction at the surface was southeasterly,
394 with no fire hotspots (solid black circle) located upwind of MACA (Fig. 9a). Without any identified
395 hotspots upwind, the model missed fire signals observed at MACA on July 3 2013.

396 Flight #0703 was a night mission targeting power plants in Missouri and Arkansas. The flight
397 path is shown in Fig. 9b and is colored by measured CH_3CN concentration. In order to highlight CH_3CH
398 concentrations above 400 ppt in the measurements, CH_3CN concentrations below 400 ppt was
399 represented by black dots. During the flight, 16 measurements of acetonitrile concentration above 400
400 ppt were observed and the maximum was 3227.9 ppt. These observations were located over
401 northwestern Tennessee and close to the borders of Kentucky, Illinois, Missouri and Arkansas. Except
402 for one observation, the flight ASL was between 500 m and 1000 m.

403 Enhancements of CO and OC were also measured concurrently with CH_3CN . Figures 9c and 9d
404 show scatter plots for CH_3CN versus CO and OC, respectively. Measured CH_3CN was highly correlated to
405 both measured CO and OC, with linear correlation coefficients (R^2) of 0.83 and 0.71, respectively. The
406 $\Delta\text{CH}_3\text{CN}/\Delta\text{CO}$ ratio is around 2.7 (ppt/ppb) --- consistent with findings of other measurements over
407 California in 2002 when a strong forest fire signal was intercepted by aircraft (de Gouw et al., 2003). The
408 $\Delta\text{CH}_3\text{CN}/\Delta\text{CO}$ ratio was around 6.85 (ppt/(mg m^{-3})) ---- in the range of biomass burning analyses in
409 MILAGRO (Megacity Initiative Local and Global Research Observations) (Aiken et al., 2010).



Figure 9e shows model simulated ΔCO with peaks at AGL below 3000 m. Fire signals showed substantial influences on aircraft measurement at around 5 UTC. However, clear fire signals between 2 UTC and 3 UTC were observed based on prior CH_3CN analysis. The model either predicted insufficient fire emission influences or missed it. FMS score on July 3 was 30%. Figure 9f shows that CMAQ did not predict plumes where the HMS plume analysis exhibited several dense smoke plumes. As NOAA Smoke Text Product (<http://www.ssd.noaa.gov/PS/FIRE/DATA/SMOKE>) described on its July 03 0501 UTC report: a smaller very dense patch of remnant smoke, analyzed earlier the same day over southern Missouri, drifted southward into Arkansas.”

The reasons the model missed these fire observations were not clear. Figures 10, 11a and 11b suggest a few clues. Figure 10 is a backward trajectory analysis plot for the observations obtained during the SENEX flight on July 3 with CH_3CN measured concentration above 400 ppt. Both the transect and flight altitude of the air parcels clearly showed those measurements were most likely influenced by the nearby pollution sources. Figure 11a illustrates the locations of fire used in the CMAQ simulation. It is noted that hmsysplit.txt is input into BlueSky after HMS quality control (Fig. 1). There were several hotspots around the region where the IMPROVE site MACA was located and where the SENEX flight overpassed. Our fire simulation system might have underestimated smoke emissions from those fires. Other explanation was from Fig. 11b, which illustrated hotspots in hmx.txt. In hmx.txt --- showing every detected fire spots by HMS before quality control. Comparing Fig. 11a with 11b, there were clusters of fire spots in the central U. S. especially in West Tennessee. However, those spots were removed during the HMS quality control process because there were no associated smoke plumes visible. In most of times, those fires were believed to be small sized fires such as from agriculture fires or prescribed burns. For this case, there seem to have been thin clouds overhead and thicker clouds in the vicinity, (<http://inventory.ssec.wisc.edu/inventory/image.php?sat=GOES-13&date=2013-07->



03&time=16:02&type=Imager&band=1&thefilename=goes13.2013.184.160147.INDX&coverage=CONUS
&count=1&offsetz=0), so it would be hard to differentiate smoke from clouds by satellite observations

CONCLUSIONS

In support of the NOAA SENEX field experiment in June-July 2013, simulations were conducted including smoke emissions from fires. In this study, a system accounting for fire emissions in a chemical transport model is described, including a satellite fire detecting system (HMS), a fire emission calculation model (BlueSky), a pre-processing of fire emissions (SMOKE), and simulation over the SENEX domain by CMAQ. The focus of this work is to evaluate the system's capability to capture fire signals identified by multiple observation data sets. These data sets included IMPROVE ground station observations, satellite observations (HMS plume shapefile and ASDTA) and airborne measurements from the SENEX campaign.

For IMPROVE data, potential fire signals were identified by measured potassium concentrations in $PM_{2.5}$. Fire identifications in CMAQ rely on its predicted ΔCO and the difference between simulations with and without fire emissions. Three out of four observed fire signals were captured by CMAQ simulations. For HMS smoke plume shapefiles that were manually plotted by analysts to represent the regions impacted by smoke, we used FMS to calculate the percentage of its overlapping with CMAQ predicted smoke plumes. FMS averaged 22% over forty days of the SENEX campaign. In terms of fire smoke impacts on ΔAOD , both ASDTA and CMAQ showed similar patterns that were compared with HMS plume shapefile analysis. In terms of measured CH_3CN , a biomass burning plume tracer, both SENEX aircraft in-flight measurements and CMAQ simulations captured signatures of long range transport of fire emissions.

Generally, using HMS-detected fire hotspots and smoke data was useful for predictions of fire impacts and their evaluation. The HMS-BlueSky-SMOKE-CMAQ fire simulation system, which is also used



455 in NAQFC, was able to capture most of the fire signals detected by multiple observations. However, the
456 system failed to identify fire cases on June 17 and July 3 2013 -- thereby demonstrating two problems
457 with the simulation system. One identified problem was the lack of a dynamical fire LBC outside the
458 CONUS domain to represent the inflows of strong fire signals originating from outside the simulation
459 domain. Secondly, the HMS quality control procedure eliminated fire hotspots that were not associated
460 with visible smoke plumes leading to an underestimation.

461 We were keen on understanding and quantifying the various uncertainties and observational
462 constraints of this study therefore the following rules of thumb were observed: (1) A holistic evaluation
463 approach was adopted so that the fire smoke algorithm was interpreted as a single entity to avoid
464 impasse arose by uncertainties specific to the different components in the system, (2) Analysis
465 conclusion applicable to the entire simulation period was drawn so that the episodic characteristics of
466 the cases embedded in the simulation were averaged and generalized. This new methodology may
467 benefit NAQFC, (3) We took advantage of the multiple perspectives of the observation systems that
468 offered a wide spectrum of temporal and spatial variabilities intrinsic to the systems, and (4) We were
469 intentional to be conservative in discarding data so that we maximized the sampling pool for statistical
470 analysis and avoided unwittingly discarding poorly simulated cases, good out-layers, and weak sparse
471 but accurate signals.

472 Quantitative evaluation of fire emissions and their subsequent influences on ozone and
473 particulate matter in this fire and smoke prediction system is challenging. Future work includes applying
474 these findings to the NAQFC and improving the NAQFC system's capabilities to simulate fires accurately.



475 **Code Availability**

476 The source code used in this study is available online at
477 <http://www.nco.ncep.noaa.gov/pmb/codes/nwprod/cmaq.v5.0.2>.

478 **Acknowledgements & disclaimer**

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480 grant NNH14AX881. The authors are thankful to Dr. Joost De Gouw and Dr. Martin G. Graus of the Earth
481 System Research Laboratory, NOAA for sharing the SENEX campaign data used in this study. Although
482 this work has been reviewed by the Air Resources Laboratory, NOAA and approved for publication it
483 does not necessarily reflect their policies or views.

484 **Figures:**

485 Figure 1, Fire emission calculation and smoke plume simulation algorithm.

486 Figure 2, in 4km SENEX domain, (a): the contribution (%) of CO emission from fires occurred inside the
487 SENEX domain; (b): the contribution (%) of CO flux flowing into the SENEX domain from its boundary
488 caused by fires burning outside the SENEX domain but inside the CONUS domain.

489 Figure 3, simulated ΔCO (ppb) extracted along SENEX flight path.

490 Figure 4, ΔCO (>2.0 ppb) simulated in SENEX domain on June 24 2013. The solid circle is detected fire
491 hotspots by HMS. The open triangle represents IMPROVE sites.

492 Figure 5, FMS (Figure of Merits in Space) (%) from June 11 to July 19 in 2013 during SENXE experiment.

493 Figure 6, HMS observed plume shape versus CMAQ predicted plume shape on (a): July 6 2013; (b): June
494 17 2013; The light blue shading represents modeled plume shape (defined as total column ΔCO) and the
495 thin dash line and emboldened green lines encircle areas representing HMS-derived light and strong
496 influenced plume shape, respectively. (c): HMS observed fire hotspots (red) and plume shapes (white)
497 (<http://ready.arl.noaa.gov/data/archives/fires/national/arcweb>) on June 17, 2013.

498 Figures 7, GOES detected AOD influenced by fires using ASDTA diagnose method. Color-shaded region
499 represents the fire-smoke influenced areas and the color denotes the magnitude of the retrieved AOD
500 on (a): June 14 2013; (d): June 25 2013; ΔAOD (with-fire – without-fire) simulated in CMAQ on (b): June



501 14 2013; (e): June 25 2013; HMS observed fire hotspots (red) and plume shapes (white)
502 (<http://ready.arl.noaa.gov/data/archives/fires/national/arcweb>) on (c): June 14 2013; (f): June 25 2013.

503 Figure 8, CMAQ simulated ΔCO vertical distributions along SENEX flight transect on (a): June 16 2013;
504 (b): July 10 2013; The x-axis label is UTC (hour) and the y-axis label is AGL (m). Two color bars represent
505 observed CH_3CN concentration (rectangle bar in ppt) and simulated ΔCO concentration (fan bar in ppb),
506 respectively.

507 Figure 9, plots for July 3 2013 case, (a): IMPROVE; (b): the flight path of SENEX #0703 colored by
508 measured CH_3CN concentration (ppt); (c): CH_3CN (ppt) vs CO (ppb); (d): CH_3CN (ppt) vs AMS_Org (mg m^{-3});
509 (e): CMAQ simulated ΔCO vertical distributions along flight transect; (f): HMS observed plume shape
510 versus CMAQ prediction.

511 Figure 10, a backward trajectory analysis for the observations obtained during the SENEX flight on July
512 03 2013 with CH_3CN measured concentration above 400 ppt.

513 Figure 11, detected fire hotspots on July 03 2013 (a): `hmxhysplit.txt`; (b): `hmx.txt`.

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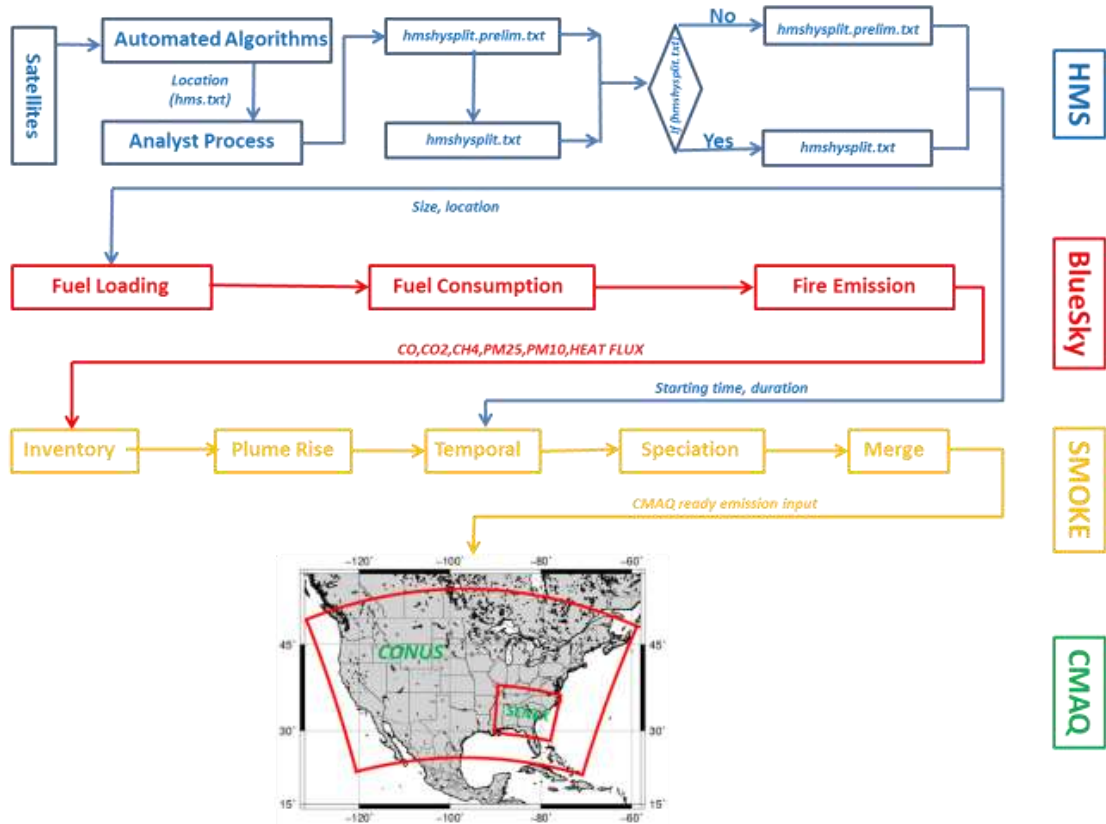


Figure 1: Fire emission calculation and smoke plume simulation algorithm

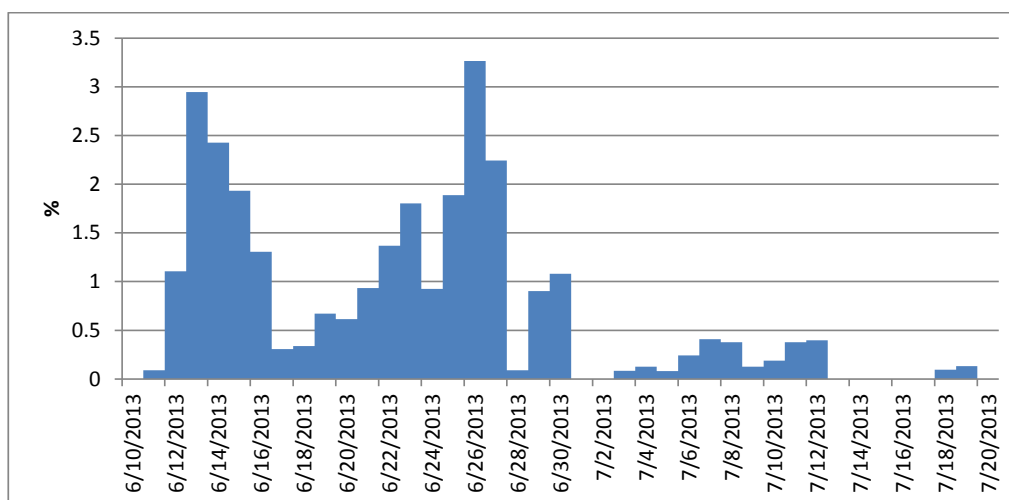


Figure 2a: the contribution (%) of CO emission from fires occurred inside the SENEX domain

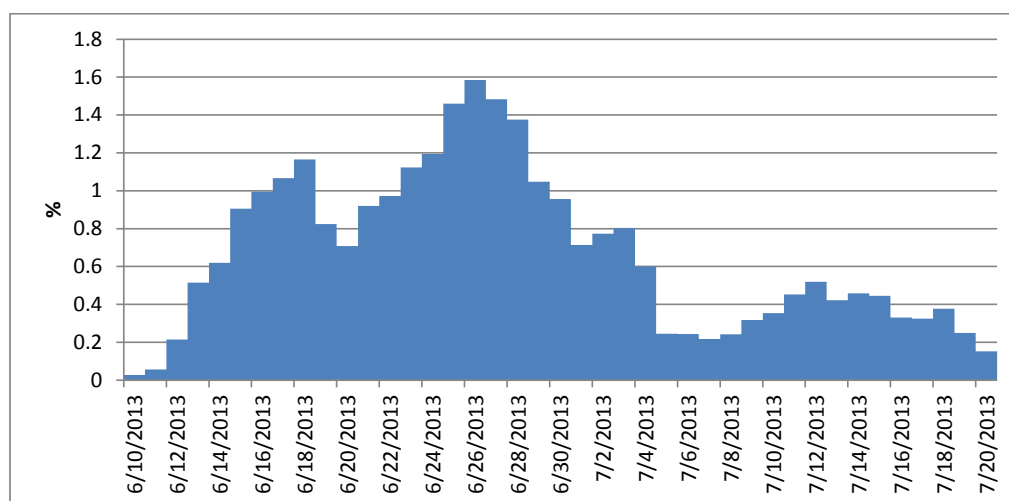


Figure 2b: the contribution (%) of CO flux flowing into the SENEX domain from its boundary caused by fires burning outside the SENEX domain but inside the CONUS domain

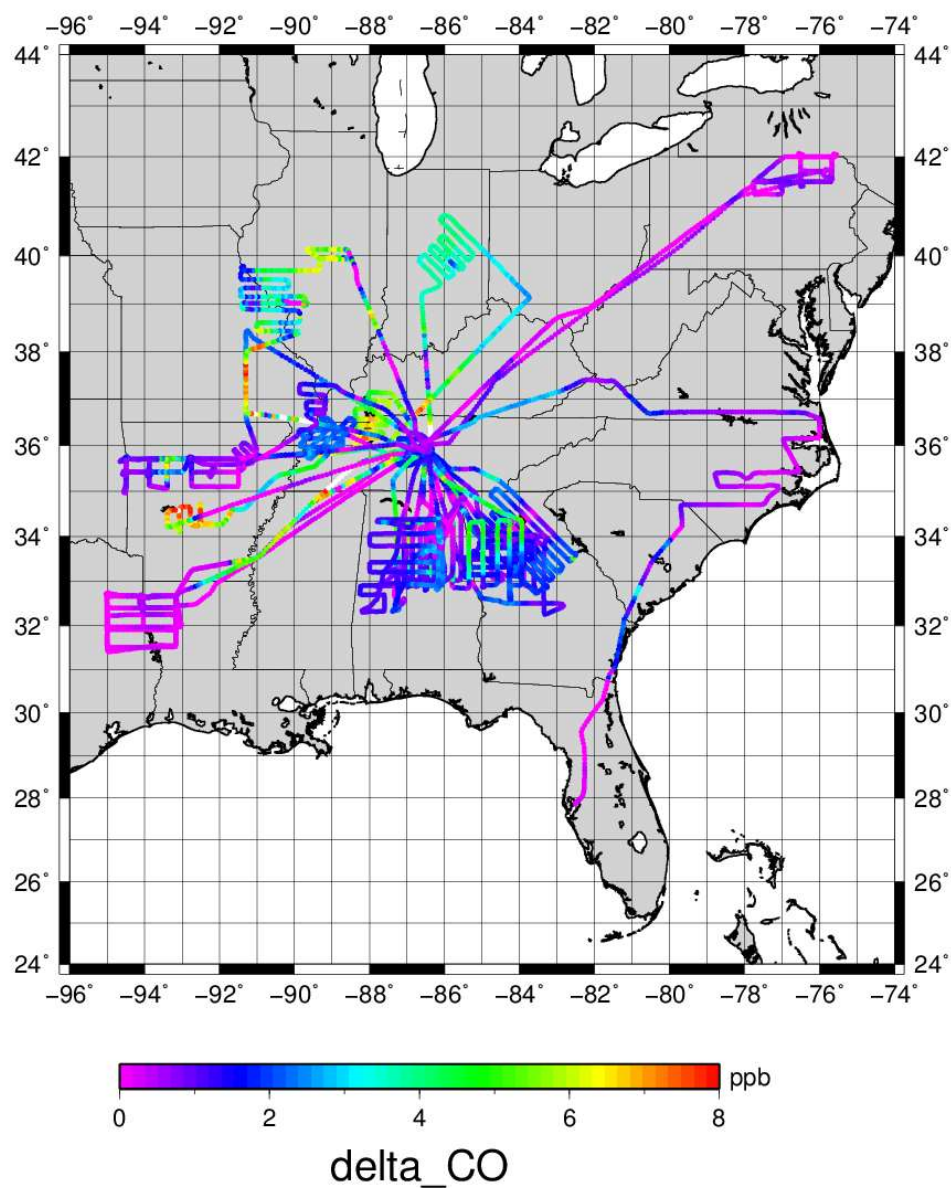


Figure 3: simulated ΔCO (ppb) extracted along SENEX flight path

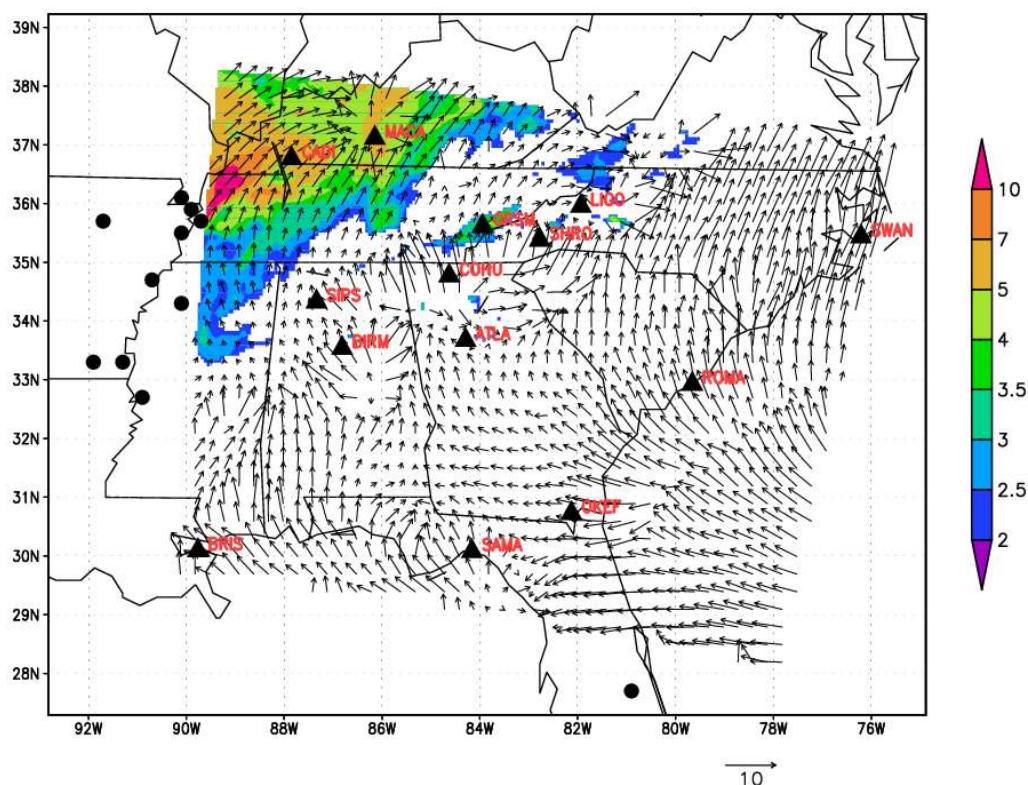
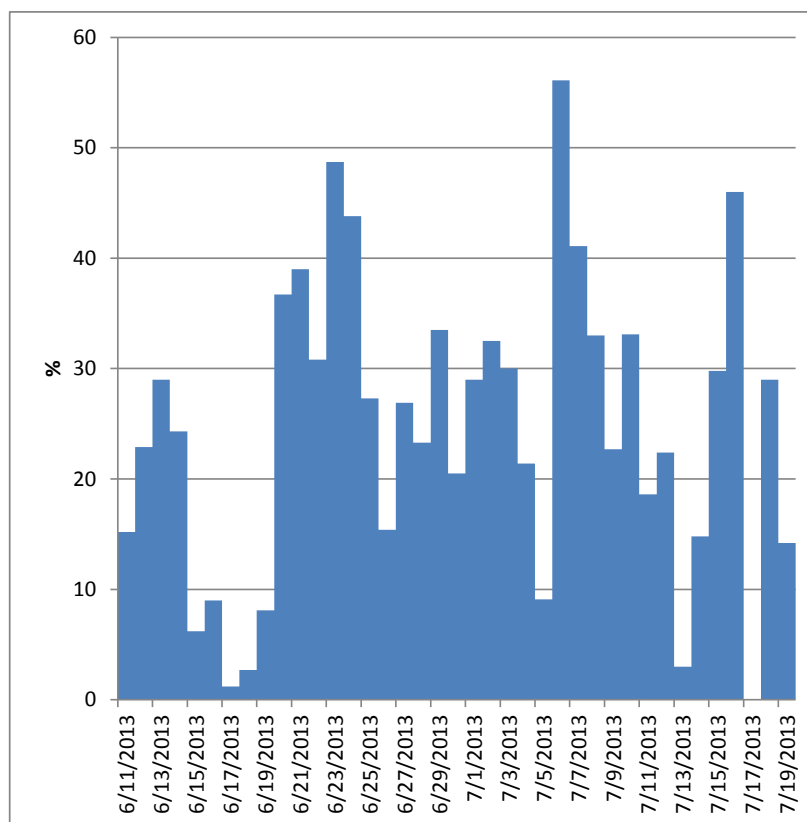


Figure 4: ΔCO (>2.0 ppb) simulated in SENEX domain on June 24 2013. The solid circle is detected fire hotspots by HMS. The solid triangle represents IMPROVE sites.



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544 **Figure 5: FMS (Figure of Merits in Space) (%) from June 11 to July 19 in 2013 during SENXE experiment**

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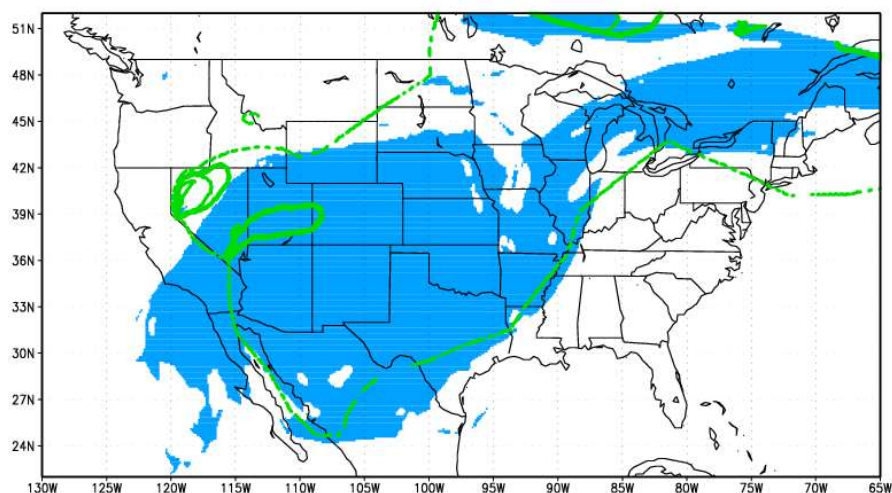


Figure 6a: HMS observed plume shape versus CMAQ predicted plume shape on July 6 2013; The light blue shading represents modeled plume shape (defined as total column ΔCO) and the thin dash line and emboldened green lines encircle areas representing HMS-derived light and strong influenced plume shape, respectively.

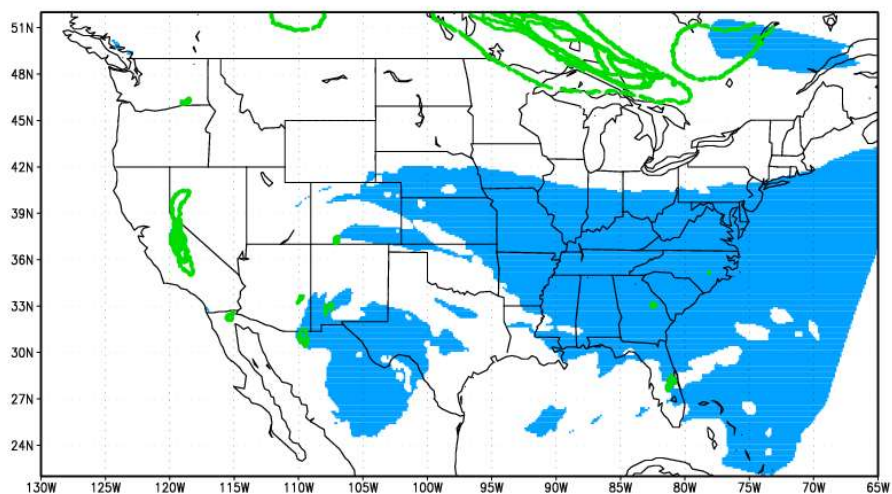


Figure 6b: on June 17 2013

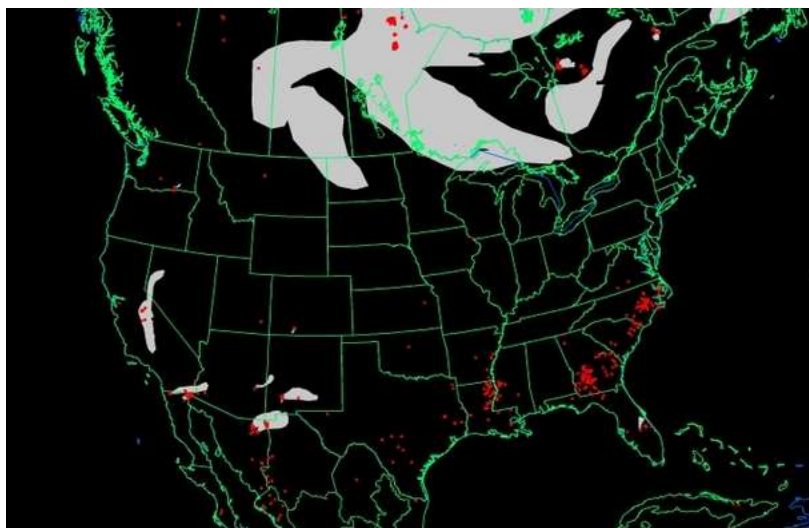


Figure 6c: HMS detected fire hotspots (red) and smoke plume shapes (white) on June 17 2013
 (<http://ready.arl.noaa.gov/data/archives/fires/national/arcweb>)

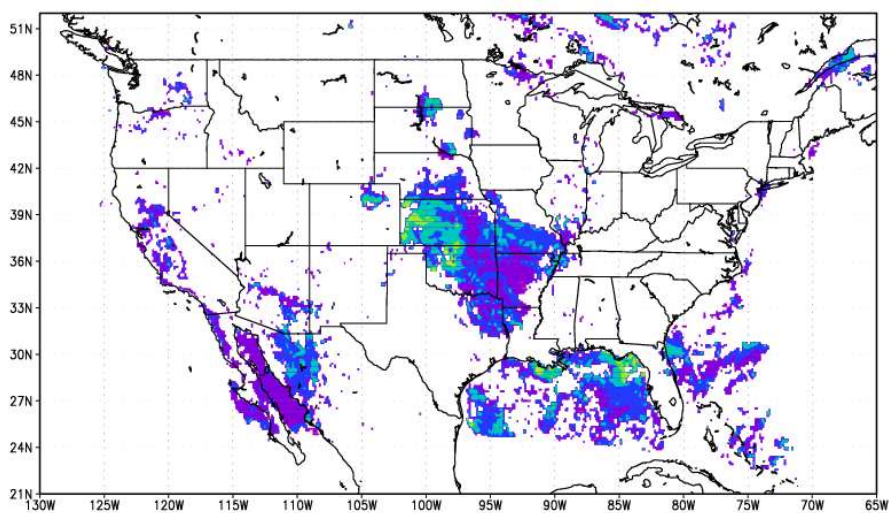
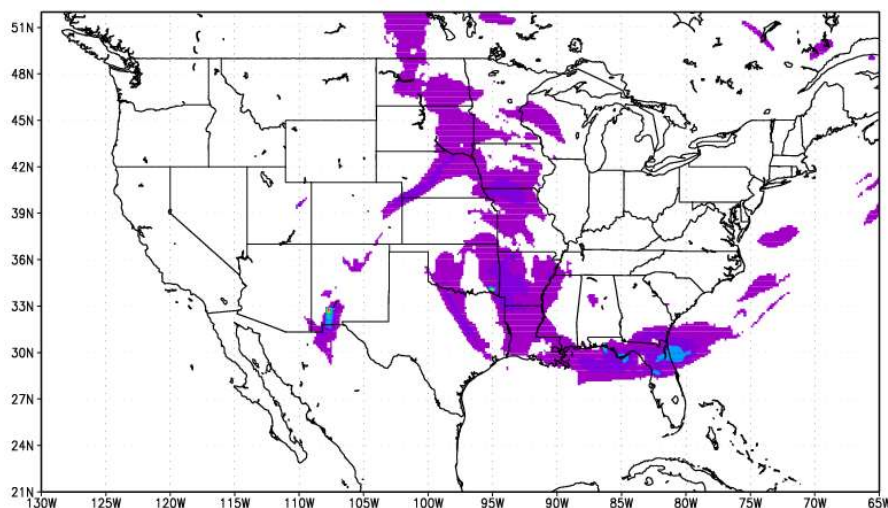


Figure 7a: GOES detected AOD influenced by fires using ASDTA diagnose method on June 14 2013.
 Color-shaded region represents the fire-smoke influenced areas and the color denotes the magnitude
 of the retrieved AOD.



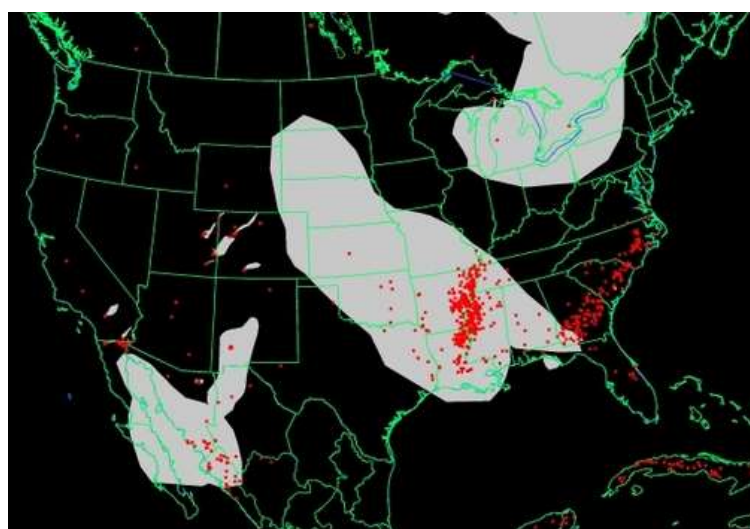
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Figure 7b: simulated ΔAOD (with-fire – without-fire) in CMAQ on June 14 2013



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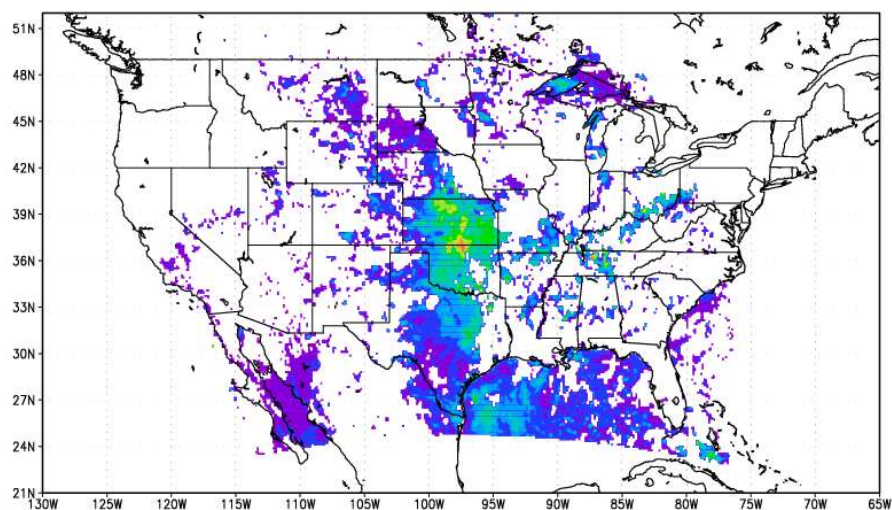
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Figure 7c: HMS detected fire hot spots (red) and smoke plume shapes (white) on June 14 2013
 (<http://ready.arl.noaa.gov/data/archives/fires/national/arcweb>)

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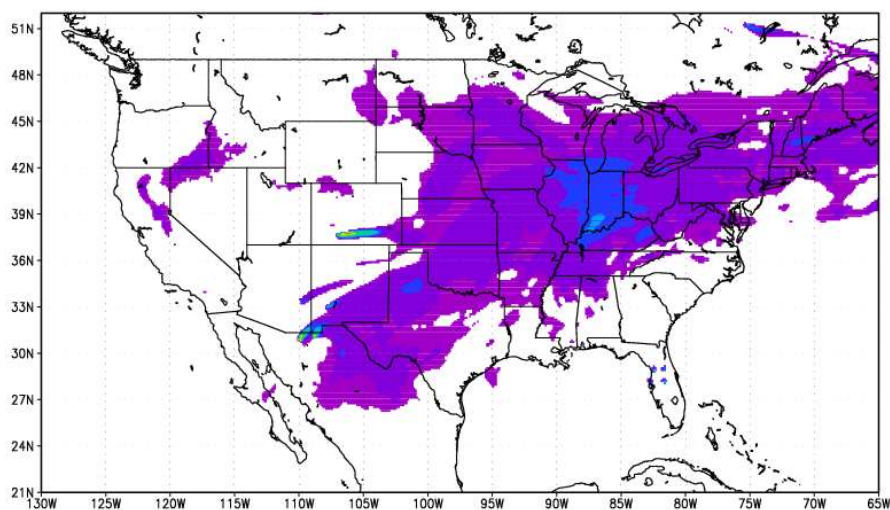


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580 **Figure 7d: GOES detected AOD influenced by fires using ASDTA diagnose method on June 25 2013.**

581 **Color-shaded region represents the fire-smoke influenced areas and the color denotes the magnitude**

582 **of the retrieved AOD.**



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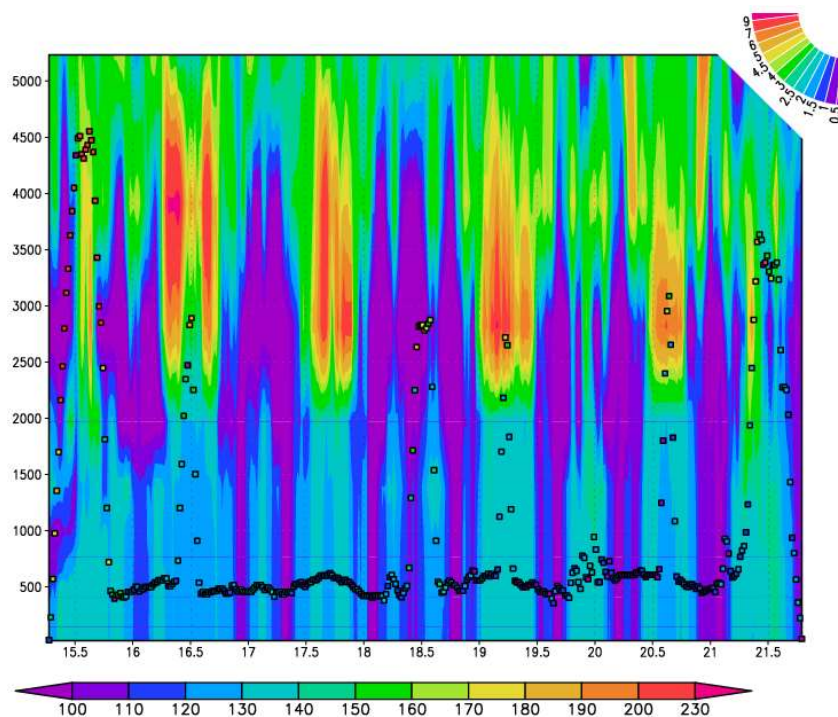
584 **Figure 7e: simulated ΔAOD (withfire – nofire) in CMAQ on June 25 2013**

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Figure 7f: HMS detected fire hot spots (red) and smoke plume shapes (white) on June 25 2013
(<http://ready.arl.noaa.gov/data/archives/fires/national/arcweb>)



592

593 **Figure 8a: CMAQ simulated ΔCO (ppb) vertical distributions along flight transect on June 16 2013. The**
 594 **x-axis label is UTC (hour) and y-axis label is AGL (m). Two color bars represent observed CH_3CN**
 595 **concentration (rectangle bar in ppt) and simulated ΔCO concentration (fan bar in ppb), respectively.**

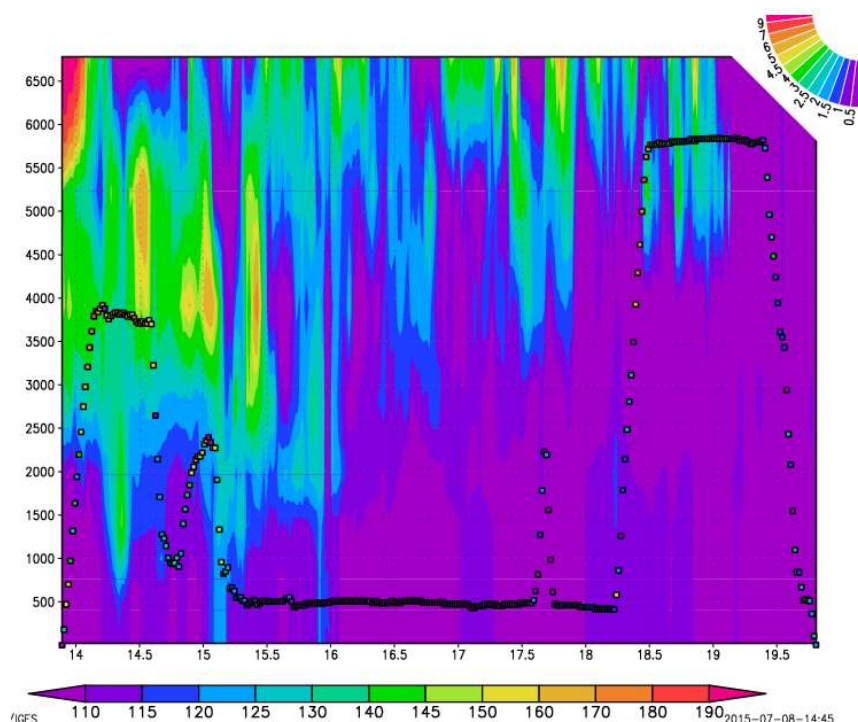
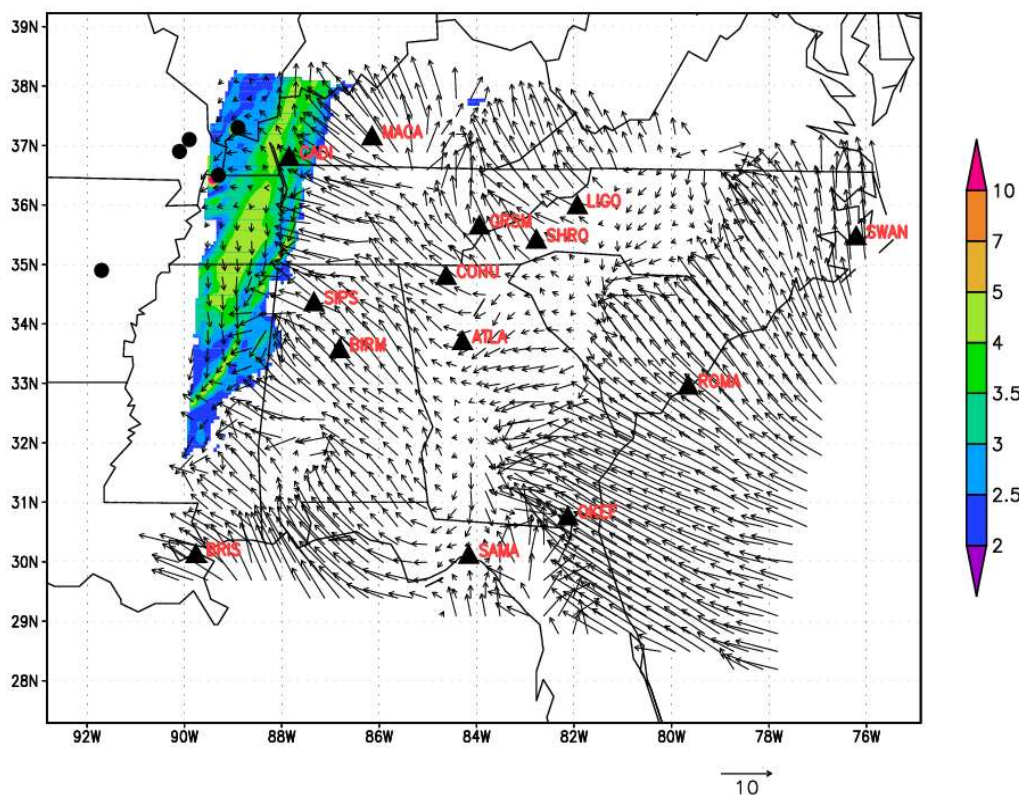


Figure 8b: CMAQ simulated ΔCO (ppb) vertical distributions along flight transect on July 10 2013. The x-axis label is UTC (hour) and y-axis label is AGL (m). Two color bars represent observed CH_3CN concentration (rectangle bar in ppt) and simulated ΔCO concentration (fan bar in ppb), respectively.



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 609 **Figure 9a: ΔCO (>2.0 ppb) simulated in SENEX domain on July 03 2013. The solid circle is detected fire**
 610 **hotspots by HMS. The solid triangle represents IMPROVE sites.**

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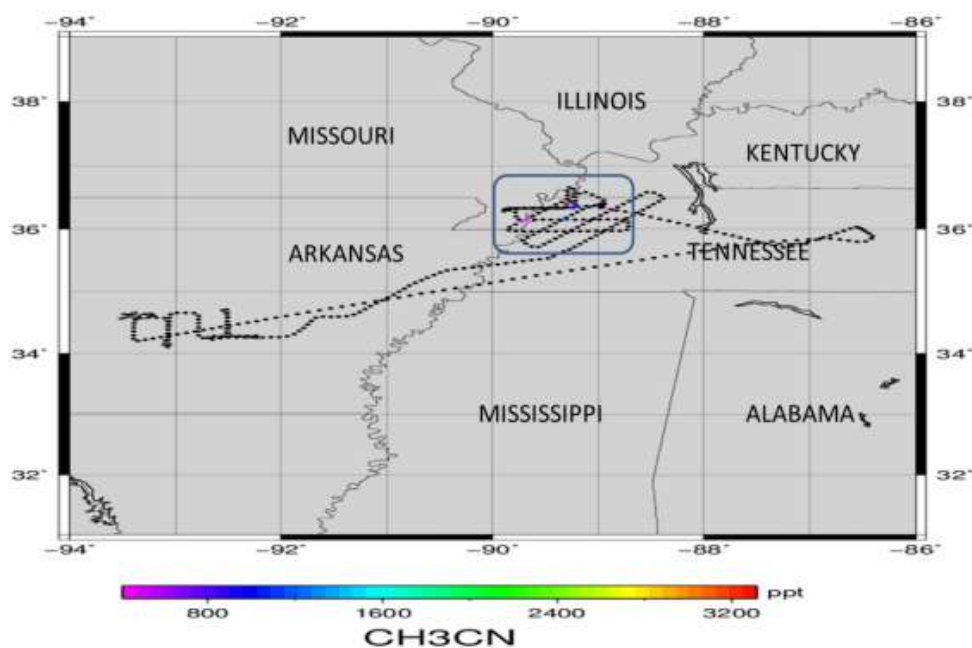


Figure 9b: the flight path of SENEX #0703, colored by measured CH₃CN concentration (ppt)

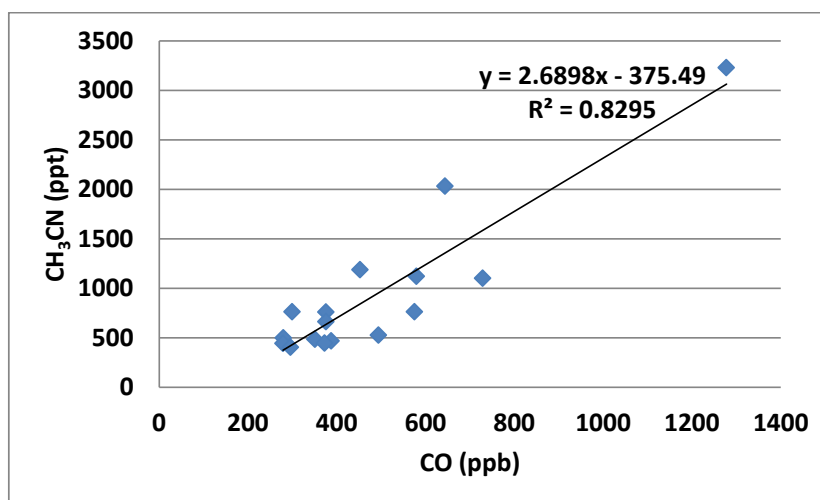


Figure 9c: CH_3CN (ppt) vs CO (ppb)

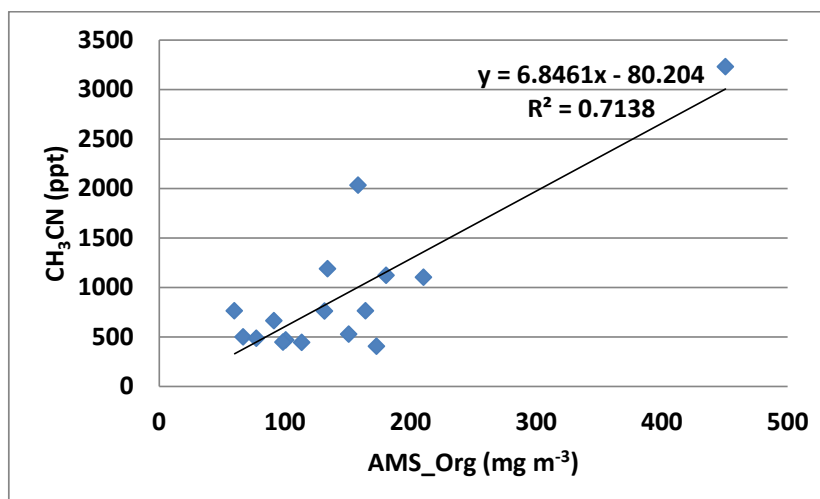


Figure 9d: CH_3CN (ppt) vs AMS_Org (mg m^{-3})

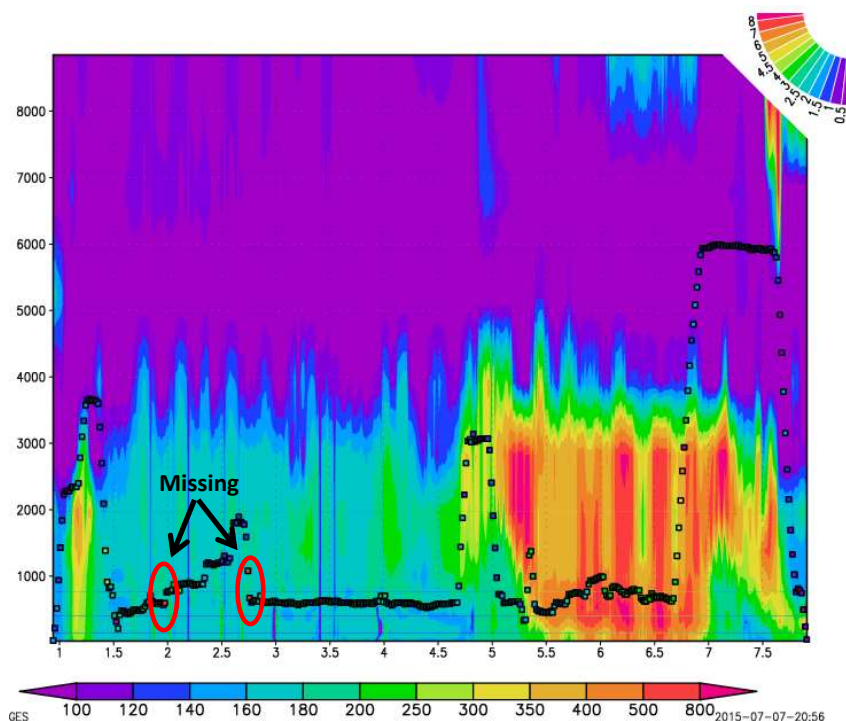
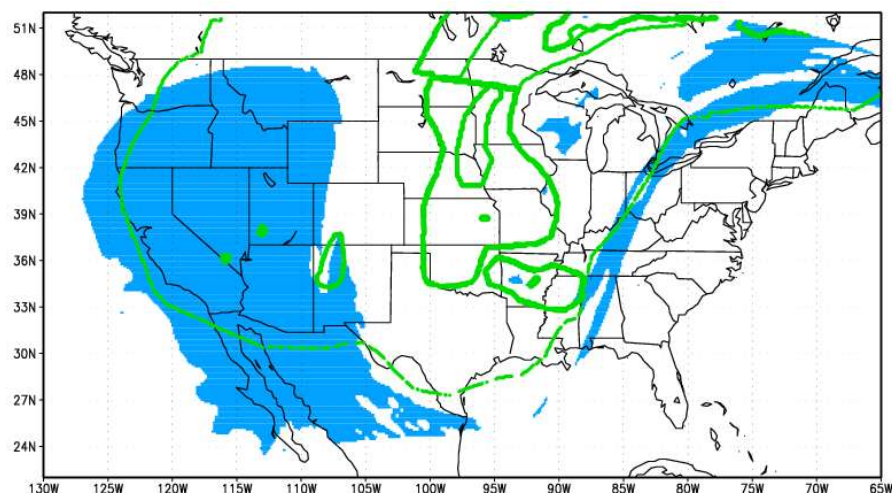


Figure 9e: CMAQ simulated ΔCO (ppb) vertical distributions along flight transect on July 03 2013. The x-axis label is UTC (hour) and y-axis label is AGL (m). Two color bars represent observed CH_3CN concentration (rectangle bar in ppt) and simulated ΔCO concentration (fan bar in ppb), respectively.



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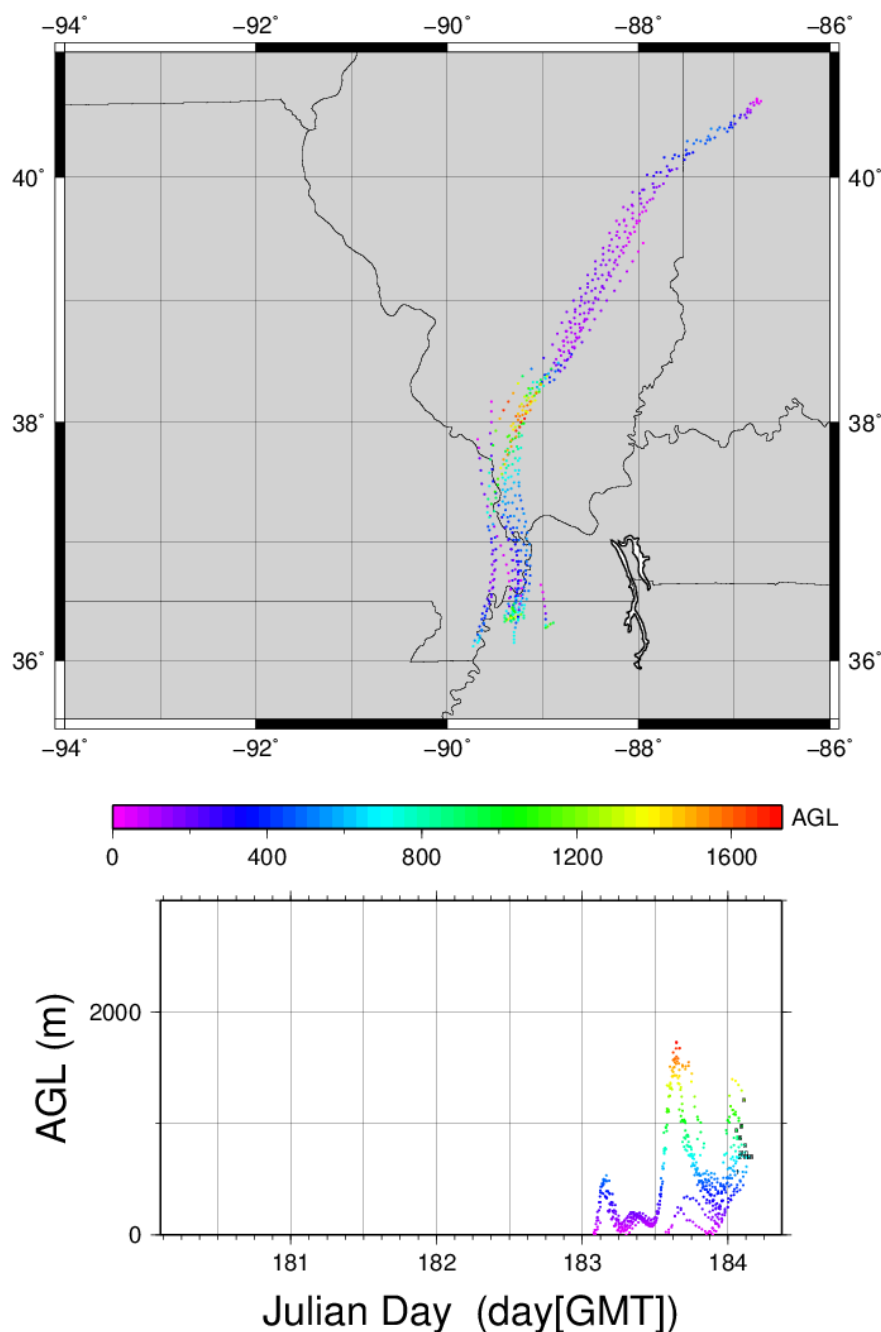
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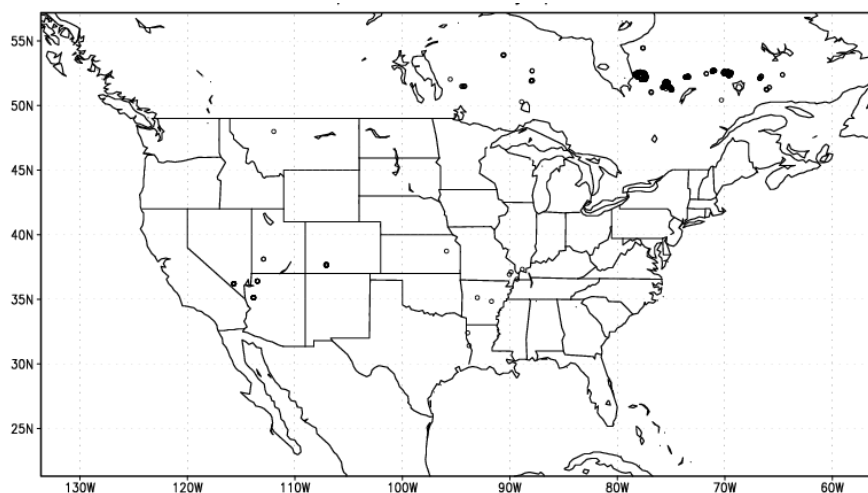
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Figure 9f: HMS plume shape versus CMAQ predictions on July 03 2013. The light blue shading represents modeled plume shape (defined as total column ΔCO) and the thin dash line and emboldened green lines encircle areas representing HMS-derived light and strong influenced plume shape, respectively.



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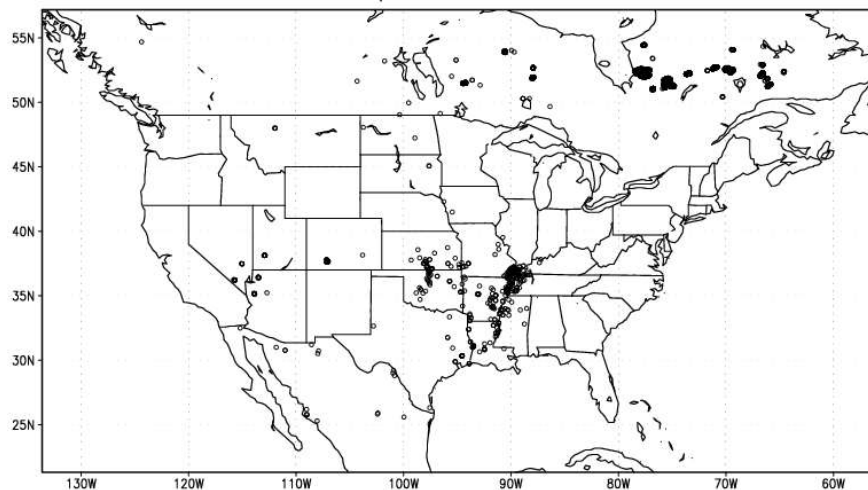
645 **Figure 10, a backward trajectory analysis for the observations obtained during the SENEX flight on July**
 646 **03 with CH₃CN measured concentration above 400 ppt.**



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Figure 11a: fire hotspots in hmxhysplit.txt on July 03 2013



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Figure 11b: fire hotspots in hmx.txt on July 03 2013

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Tables:

Table 1: observed and simulated CO (ppb) during NOAA SENEX experiment

AGL (m)	SAMPLE SIZE	OBS	OBS_MAX	Mod_withfire	Mod_nofire	ΔCO
<500	166	128.93±38.51	319.55	108.70±21.37	107.16±20.34	1.54
500~1000	3565	146.19±44.39	1277.97	108.39±19.82	106.50±18.86	1.88
1000~1500	793	125.41±28.09	299.64	100.11±15.63	98.49±14.67	1.62
1500~2000	306	119.68±23.99	265.29	100.75±17.04	99.08±15.89	1.67
2000~2500	219	111.48±19.98	286.22	99.88±17.95	98.37±16.92	1.51
2500~3000	209	111.84±19.79	295.79	97.43±12.21	95.87±11.15	1.56
3000~3500	181	109.31±16.66	197.94	89.34±12.09	88.13±11.06	1.21
3500~4000	195	110.78±14.36	140.42	92.11±10.73	90.25±9.62	1.86
4000~5000	369	89.82±19.09	138.04	80.36±10.15	79.17±9.14	1.19
5000~6000	354	102.26±22.37	209.20	78.12±7.64	76.82±6.28	1.30
6000~7000	85	87.53±17.88	115.32	73.35±4.71	70.58±2.45	2.77

Table 2: identified fire signals from IMPROVE measurements during SENEX experiment

Site	Date	Concentrations (ug m ⁻³)						Concentration/Average						Ratio	
		EC	OC	K	SOIL	NO ₃ ⁻	SO ₄ ²⁻	EC	OC	K	SOIL	NO ₃ ⁻	SO ₄ ²⁻	BC/OC	K/BC
COHU	0621	0.28	2.10	0.05	0.22	0.13	2.61	1.4	1.46	1.42	0.39	0.84	1.28	0.1331	0.1933
MACA	0624	0.45	2.34	0.09	0.26	0.24	2.76	1.85	1.58	1.82	0.48	1.19	1.24	0.1929	0.1973
MACA	0703	0.33	2.32	0.08	0.16	0.29	2.11	1.35	1.57	1.73	0.29	1.43	0.94	0.1423	0.2554
BRIS	0703	0.24	0.98	0.21	0.31	0.11	2.63	1.49	1.28	2.79	0.13	0.35	1.36	0.2458	0.8851
GRSM	0621	0.25	1.56	0.05	0.24	0.13	2.52	1.36	1.45	1.24	0.49	0.99	1.42	0.1596	0.1979



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