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

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Abstract

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

Introduction

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

48   estimation algorithm, the U.S. EPA Sparse Matrix operator Kernel Emission (SMOKE) applied for fire

49   plume rise calculations, the NOAA National Weather Service (NWS) North American Multi-scale Model

50   (NAM) for meteorological prediction and the U.S. EPA Community Multi-scale Air Quality Model (CMAQ)

51   for chemical transport and transformation. In contrast to most anthropogenic emissions, smoke

52   emissions from fires are largely uncontrolled, transient and unpredictable. Consequently, it is a

53   challenge for air quality forecasting systems such as NAQFC to describe fire emissions and their impact

54   on air quality (Pavlovic et al., 2016; Lee et al., 2017; Huang et al., 2017).

55   Southeast Nexus (SENEX) was a NOAA field study conducted in the Southeast U.S. in June and

56   July 2013 (Warneke et al., 2016). This field experiment investigated the interactions between natural

57   and anthropogenic emissions and their impact on air quality and climate change (Xu et al., 2016;

58   Neuman et al., 2016). In this work, the SENEX dataset was used to evaluate the HMS-BlueSky-SMOKE-

59   CMAQ fire simulations during the campaign period.

60   Two simulations were performed: one with and one without smoke emissions from fires during

61   the SENEX field campaign. Due to the large uncertainties in the estimates of fire emissions and smoke

62   simulations (Baker et al., 2016; Davis et al., 2015; Drury et al., 2014), the first step of the evaluation

63   focused on the fire signal capturing capability of the system. Differences between the two simulations

64   represented the impact of the smoke emissions from fires on the CMAQ model results. Observations

65   from various sources were utilized in this analysis: (i) ground observations (Interagency Monitoring of

66   Protected Visual Environments (IMPROVE)), (ii) satellite retrievals (Automated Smoke Detection and

67   Tracking Algorithm (ASDTA) and HMS smoke plume shape), and (iii) aircraft measurements (SENEX

68   campaign). Fire signals predicted by the modeling system were directly compared to these observations.

69   Several criteria have been used to rank efficacy of the observation systems for fire induced pollution

70   plumes.

Methodology

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

HMS (Hazard Mapping System)

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

       HMS first processes satellite data by using automated algorithms for each of the satellite platforms to detect fire locations (Justice et al., 2002; Giglio et al., 2003; Prins and Menzel 1992; Li et al., 2000), which is then manually analyzed by analysts to eliminate false detections and/or add missed fire hotspots. The size of the fire is represented by the number of detecting pixels corresponding to the nominal resolution of MODIS or AVHRR data. Fire starting times and durations are estimated from close inspection of the visible band satellite imagery. A bookkeeping file is generated at the end of this detection step, named "hms.txt" (Fig. 1). It includes all the thermal signal hotspots detected by the aforementioned 7 satellites. During the analyst quality control step, detected potential fire hotspots lacking visible smoke in the retrieval's HMS (RGB real-color) imagery are removed resulting in a reduced fire hotspot file called either "hmshysplit.prelim.txt" or "hmshysplit.txt" to be input into the BlueSky processing step.

94   In general, "hmshysplit.prelim.txt" and "hmshysplit.txt" are very similar, and "hmshysplit.txt" is

95   created later than "hmshysplit.prelim.txt" (Fig. 1). But the differences between "hmx.txt" and

96   "hmshysplit.txt" ("hmshysplit.prelim.txt") can be rather substantial. The reasons for differences are: 1)

97   many detected fires do not produce detectable smoke; 2) some fires/hotspots are detected only at

98   night, when smoke detection is not possible; 3) smoke emission HMS imagery is obscured by clouds thus

99   not detected by the analyst. Therefore, smoke emission occurrence provided by the HMS is a

100   conservative estimate of fire emissions.

101   By using multiple satellites the likelihood of detecting fires in HMS is robust. However, when the

102   fire geographical size is small the HMS detection accuracy dramatically decreases (Zhang et al., 2011; Hu

103   et al., 2016). Other limitations of the HMS fire detections include ineffective retrievals at nighttime and

104   under cloud cover.

BlueSky

106   BlueSky, developed by the USFS (US Forest Service), is a modeling framework to simulate smoke

107   impacts on regional air quality (Larkin et al., 2009; Strand et al., 2012). In this study, BlueSky acted as a

108   fire emission model to provide input for SMOKE (Herron-Thorpe et al., 2014; Baker et al., 2016). BlueSky

109   calculates fire emission based on HMS-derived locations (Fig. 1).

110   Fire geographical extent is reflected by the number of nearby fire pixels detected by satellites in

111   a 12-km CMAQ model grid. Fire pixels are converted to fire burning areas in BlueSky based on the

112   assumption that each fire pixel has a size of 1 km^2 and 10% of its area can be considered as burn-active

113   (Rolph et al., 2009). All fire pixels in a 12-km grid square are aggregated. BlueSky uses the following to

114   estimate biomass availability: fuel loading map is from the US National Fire Danger Rating System

115   (NFDRS) for the Conterminous US (CONUS) with the exception in western US where the HARDY set is

116   used (Hardy and Hardy 2007). BlueSky uses Emissions Production Model (EPM) (Sandberg and Peterson

117   1984), a simple version of CONSUME, to calculate fuel actually burned -- the so-called consumption

118   sums. Finally, EPM is also used in BlueSky to calculate the fire emission hourly rate per grid-cell. BlueSky

119   outputs CO, CO_2, CH_4, non-methane hydrocarbons (NMHC), total PM, $PM_{2.5}$, PM_{10} and heat flux (Fig. 1).

120   BlueSky does not iteratively recalculate fire duration according to the modeled diminishing fuel

121   loading or the modeled fire behavior. In the aggregation process, when there is more than one HMS

122   point in a grid cell which have different durations, all points in that grid cell would be assigned the

123   largest duration in all points. For an example, if there were 3 HMS points that had durations of 10, 10

124   and 24 hours, the aggregation would include 3 points (representing 3 km^2) assigned with 24 hour

125   duration to all of the 3 HMS points.

126   HMS has no information about fuel loading. BlueSky uses a default fuel loading climatology over

127   the eastern US. BlueSky uses an idealized diurnal profile for fire emissions. Uncertainties in fire sizes,

128   fuel loading and fire emission rates lead to large uncertainties in wildland smoke emissions (Knorr et al.,

129   2012; Drury et al., 2014; Davis et al., 2015).

130   **SMOKE**

131   In SMOKE (Sparse Matrix Operator Kernel Emission), the BlueSky fire emissions data in a

132   longitude-latitude map projection are converted to CMAQ ready gridded emission files (Fig. 1). Fire

133   smoke plume rise is calculated using formulas by Briggs. The heat flux from BlueSky and NAM

134   meteorological state variables are used as input (Erbrink 1994). The Briggs' algorithm calculates plume

135   top and plume bottom, between plume top and bottom the emission fraction is calculated layer by layer

136   assuming a linear distribution of flux strength in atmospheric pressure. For model layers below the

137   plume bottom the emission fraction is assumed to be entirely in the smoldering condition as a function

138   of the fire burning area.

139   A speciation cross-reference map was adopted to match BlueSky chemical species to that in

140   CMAQ using the U.S. EPA Source Classification Codes (SCCs) for forest Wildfires

141   (https://ofmpub.epa.gov/sccsearch/docs/SCC-IntroToSCCs.pdf). The life-span of fire is based on the HMS

142   detected fire starting time and duration. During fire burning hours a constant emission rate is assumed.

143   This constant burn-rate has been shown to be a crude estimate (Saide et al., 2015; Alvarado et al.,

144   2015). Other uncertainties include plume rise (Sofiev et al., 2012; Urbanski et al., 2014; Achtemeier et

145   al., 2011) and fire-weather (fire influencing local weather).

CMAQ

147   The CMAQ version 4.7.1 was used. The CB05 gas phase chemical mechanism (Yarwood et al.,

148   2005) and the AERO5 aerosol module (Carlton et al., 2010) were chosen. Anthropogenic emissions were

149   based on the U.S. EPA 2005 National Emission Inventory (NEI) projected to 2013 (Pan et al., 2014),

150   Biogenic emissions (BEIS 3.14) were calculated in-line inside CMAQ.

Simulations

152   The NAM provided meteorology fields to drive CMAQ (Chai et al., 2013). NAM meteorology is

153   evaluated   daily   and   results   (BIAS   and   RMSE   etc.)   are   posted   on:

154   "http://www.emc.ncep.noaa.gov/mmb/mmbpll/mmbverif/". The simulation domain is shown in Fig. 1.

155   It includes two domains: (i) a 12-km domain covering the Continental U.S. (CONUS); and (ii) a 4km

156   domain covering the Southeast U. S. where the majority of SENEX measurements occurred. Lateral

157   boundary conditions (LBC) used in the smaller SENEX domain simulation were extracted from that from

158   the CONUS simulations. Four scenarios were simulated: CONUS with fire emissions, CONUS without fire

159   emissions, SENEX with fire emissions and SENEX without fire emissions.

160   There were several differences in system configuration between the NAQFC fire smoke

161   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. 2019 (manuscript in preparation)). The

165   analytical run is a 24-hour retrospective simulation using yesterday's meteorology and fire emissions to

166   provide initial conditions for today's forecast. The forecasting run is a 48-hour predictive simulation

167   using yesterday's fire emissions, assuming fires with duration of more than 24 hours are projected as

168   continued fires.. The "with-fire" simulation in this study is exactly identical to the analysis run in NAQFC.

169   **Evaluations**

170   Carbon monoxide (CO) has a relatively long life time in the air and is emitted by biomass

171   burning. CO was used as a fire tracer in the prediction. The CO difference (ΔCO) between CMAQ

172   simulations with and without fire emissions was used as the indicator of fire influence. For additional

173   observations included: potassium (K) collected at the IMPROVE (Interagency Monitoring of Protected

174   Visual Environments) sites within the SENEX domain; acetonitrile (CH_3CN) measured from the SENEX

175   campaign flights; and fire plume shape detected by the HMS analysis as real fire signals.   The

176   enhancement in ΔCO concentration due to fire was directly compared with those signals. At the same

177   time, ΔAOD (Aerosol Optical Depth) from CMAQ ("with-fire" simulated concentration minus that with

178   "without-fire") was also used as fire indicator when compared with smoke masks given by the ASDTA

179   (Automated Smoke Detection and Tracking Algorithm).

180   It is almost impossible to assess the uncertainty of each specific smoke physical process. In each

181   modeling step in HMS, BlueSky, SMOKE and CMAQ, the modeling system accrues uncertainties. Such

182   uncertainties were likely cumulative and might lead to larger error in succeeding components

183   (Wiedinmyer et al., 2011). For an example, heat flux from BlueSky influenced plume rise height in

184   SMOKE and consequently influenced plume transport in CMAQ. It is also noteworthy that when

185 modeled ΔCO was against measured K or CH₃CN, the objective was to search for enhancement signals

186 resulting from fires but not aiming to account for proportional concentration changes in the tracers in

187 the event of a fire. Attempting to account for CMAQ simulation uncertainties in surface ozone and

188 particulate matter as a function of smoke emissions from fires was difficult. Neither was it the objective

189 of this study. Rather, the purpose of this study is to focus on analyzing the capability of the HMS-

190 BlueSky-SMOKE-CMAQ modeling system to capture fire signals.

191   The SENEX campaign occurred in June and July and our model simulations were from June 10 to

192 July 20, 2013. Throughout the campaign all available observation datasets were used including ground-,

193 air- and satellite-based acquired data. Each dataset had its unique characteristics and linking them

194 together gave an overall evaluation. At the same time, in each dataset our evaluations included as many

195 as possible observed fire cases. Both well-predicted and poorly-predicted cases are presented to

196 illustrate potential reasons responsible for the modeling system's behavior.

Results and Discussions

197

Observed CO versus modeled CO in SENEX

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199   Table 1 lists observed and modeled CO vertical profiles for the "with-fire" and "without-fire"

200 cases during the SENEX campaign. Observed CO concentrations between the surface and 7 km AGL

201 (Altitude above Ground Level) in the SENEX domain area remained greater than 100 ppb during all 40

202 days of the campaign. The highest CO concentrations were measured closer to the surface. The

203 maximum measured CO concentration of 1277 ppb was observed during a flight on July 03 at an ASL

204 (Altitude above Sea Level) of 974 m. In this flight strong fire signals were observed but the fire

205 simulation system missed those signals as discussed below.

206   CO concentrations were underestimated by the model in almost all cases even when the model

207   captured CO contribution from fire emissions spatio-temporarily. Mean ΔCO in each height interval was

208   usually above 1.5 ppb but less than 2.0 ppb. Fig. 2a shows the contribution of total CO emissions from

209   fires which occurred inside the SENEX domain over the simulation period. The maximum CO emissions

210   contribution from fires was about 3% during the campaign. In most of those days fire emission

211   contributions in SENEX were less than 1%. The averaged contribution during those 40 days was 0.7%.

212   Fig. 2b shows the contribution of CO flowing into the SENEX domain from its boundary caused by fire

213   outside the SENEX domain but inside the CONUS domain (Fig. 1). The averaged fire contribution to CO

214   from outside the SENEX domain was 0.67%. CO influenced by fire emission in June is greater than that in

215   July.

216   During the field experiment the general lack of large fires made evaluation of modeled fire

217   signature difficult since it was easier to capture large fire signals than the smaller fires. We postulated

218   that a clear fire signal simulated in the HMS-BlueSky-SMOKE-CMAQ system could be indicated by ΔCO

219   significantly larger than its temporal averages resulted by fires originated from inside and/or outside the

220   SENEX domain. For an example, a clear fire signal between 500 m and 1000 m AGL was indicated by ΔCO

221   across those altitudes and when the concentration of ΔCO was above 2.0 ppb based on the campaign

222   duration averaged CO concentration of about 150 ppb as well as on within the SENEX domain and

223   outside of the SENEX domain fire contributions to CO (150*(0.007+0.0067) =2.0).

224   Figure 3 displays the simulated ΔCO extracted along SENEX flight path during the SENEX

225   campaign. The modeled concentration showed that the fire impacts on SENEX were not negligible

226   despite a lack of larger fire events as shown in Fig. 2a and 2b during the SENEX campaign period. That

227   confirmed the importance of evaluating the fire simulation system in an air quality model. Unless a

228   model is able to predict fire signals correctly it is useless for modelers to discuss fire effects on chemical

229   composition of the atmosphere. A detail of how model caught or missed or falsely predicted fire signals

230   during the SENEX campaign and a comparison of ΔCO versus CH_3CN will be discussed in the follow

231   discussion.

232   **IMPROVE**

233   The Interagency Monitoring of Protected Visual Environments (IMPROVE) is a long term air

234   visibility monitoring program initiated in 1985 (http://vista.cira.colostate.edu/Improve/data-page). It

235   provides 24-h integrated particulate matter (PM) speciation measurements every third day (Malm et al.,

236   2004; Eatough et al., 1996). The IMPROVE dataset was chosen for this analysis because it included K

237   (potassium), OC (organic carbon) and EC (elemental carbon), important fire tracers. IMPROVE monitors

238   are ground observation sites likely influenced by nearby fire sources.

239   There were 14 IMPROVE sites in the SENEX domain (Fig. 4). Potential fire signals were identified

240   by using CMAQ modeled ΔCO and IMPROVE observed K. However, in addition to fires K has multiple

241   sources such as soil, sea salt and industry. Co-incidentally fires should also produce enhanced EC and OC

242   concentrations, a fire signal should reflect above-average values for EC, OC, and K.   EC, OC and K

243   observations that were 20% above their temporal averages during the SENEX campaign were used as a

244   predictor for fire event identification. Meanwhile, co-measured NO_3^- and SO_4^{2-} concentrations are less

245   than 1.5 times of their respective temporal averages for screening out data with industrial influences.

246   Lastly, a third predictor was employed so that concentrations of other soil components besides K should

247   be below their temporal average to eliminate conditions of spikes in K concentration due to dust. With

248   these three criteria the IMPROVE data was screened for fire events (See Table 2).

249   Five fire events were observed at four IMPROVE sites. Table 2 lists measured EC, OC, NO_3^-, K, soil

250   and SO_4^{2-} concentrations (μg m^{-3}) and their ratios to averages. BC versus OC and K versus BC ratios were

251   also calculated and listed in Table 2 to illustrate the application of our criteria. It was found that except

252   for monitor BRIS, all other sites (COHU, MACA and GRSM) had BC/OC and K/BC ratios comparable to the

253   ratios of the same quantities due to biomass burning reported by other researchers (Reid et al., 2005;

254   DeBell et al., 2004). BRIS is a coastal site likely influenced by sea salts (Fig. 4).

255   For the four identified fire cases, ΔCO as a modeled fire tracer around the IMPROVE site was

256   plotted. Fire signals on June 21 at COHU and GRSM and on June 24 at MACA were reproduced in model

257   simulation. The June 24 MACA case was used as an example (see Fig. 4).On June 24, 2013, detected fire

258   spots were outside the SENEX domain, but SSW wind blew smoke plumes into the SENEX domain and

259   affected modeled CO in MACA. Modeled ΔCO in MACA was 5 ppb.

260   Another IMPROVE site located upwind of MACA, CADI, was also potentially under the influence

261   of that fire event; however, data from CADI on June 24 did not indicate a fire influence, possibly due to

262   the frequency of IMPROVE sampling that eluded measurement or that the smoke plume was

263   transported above the surface in disagreement with what was modeled. Within the four fire cases

264   identified by the IMPROVE data during SENEX (Tab. 2), the model successfully captured three out of four

265   events. The model missed fire signal on July 3 at MACA. The model missed the fire signal on July 3 at

266   MACA. The following section is dedicated to the July 3 SENEX flight.

267   **Plume Spatial Coverage**

268   HMS determines fire hotspot locations associated with smoke and upon incorporating the

269   smoke plume shape information from visible satellite images. HMS provides smoke plume shapefiles

270   over much of North America, which is a two-dimensional smoke plume spatial depiction collapsing all

271   plume stratifications to a satellite eye-view. For modeled plumes, we integrated modeled ΔCO by

272   multiplying the layer values with the corresponding CMAQ model layer thicknesses and air density to

273   derive a simulated smoke plume shape. HMS-derived smoke plume shape versus CMAQ predicted

274   smoke plume shape was then used to evaluate the fire simulation.

275   Figure of Merits in Space (FMS) (Rolph et al., 2009) is a statistic for spatial analysis and was

276   calculated as follows:

$$FMS = \frac{Area\_hms \ \cap \ Area\_cmaq}{Area\_hms \ \cup \ Area\_cmaq} \ X \ 100\%$$

277   Where Area_hms represents area of grid cells influenced by fire emission over CONUS detected by HMS

278   and Area_cmaq represents area of grid cells over CONUS identified by model prediction. In general, a

279   higher FMS value indicates a better agreement between the observed and modeled plume shape (Rolph

280   et al., 2009).

281   Figure 5 summarizes FMS during the SENEX campaign. Average FMS was 22% with its maximum

282   at 56% on July 6 and minimum at 1.2% on June 17 2013. Figure 6a exhibits HMS detected smoke plume

283   and CMAQ calculated smoke plume over CONUS on July 6. The FMS score was 56% meaning that the

284   modeled plume shape was consistent with that of HMS. However, HMS-BlueSky-Smoke emissions

285   system might have underestimated the intensive fire influence areas along the border of California and

286   Nevada. Subsequently, the model also under-predicted its associated influence in North Dakota, South

287   Dakota, Minnesota, Iowa and Wisconsin.

288   Figure 6b exhibits the worst case on June 17 2013 in terms of resulting with a FMS score at 1.2%.

289   Two reasons led to this: (i) CMAQ missed fire emissions from Canada. Those fire sources located outside

290   the CONUS modeling domain and our simulation system used a climatologically-based static LBC;

291   Secondly on June 17, there were a lot of fire hotspots in the Southeastern U.S., i.e., in Louisiana,

292   Arkansas and Mississippi along the Mississippi River. Hotspots were detected but they lacked associated

293   smoke in corresponding HMS imagery (Fig. 6c). This could be due to cloud blockage or to small

294   agricultural debris clearing, burns in under-bushes or prescribed burns. These conditions prevented the

295   HMS from identifying fires and hence emissions were not modeled for those sources.

296   It is noteworthy that the FMS evaluation contained uncertainties contributed from both

297   modeled and observed values. The calculated campaign duration and SENEX-wide averaged FMS was

298   22%. It is significantly higher than that achieved by similar analyses done by HYSPLIT (Hybrid Single

299   Particle Lagrangian Integrated Trajectory) smoke forecasting for the fire season of 2007 (6.1% to 11.6%)

300   (Rolph et al., 2009). The primary reason is that the HYSPLIT smoke simulation is accessed at the

301   invocation of a forecast cycle the HMS fire information which is already one day old due to retrieval

302   latency and cycle-queuing issues. However, our model simulation in this study was from a retrospective

303   module using current day HMS fire information. Such discrepancies have been discussed by Huang et al.

304   2019 (*manuscript in preparation*). The secondary reason is plume rise: despite both the HYSPLIT and

305   CMAQ fire plume rise were estimated by the Briggs' equation, the HYSPLIT plume rise was limited to

306   75% of the mixed layer height (MLH) at daytime and two times MLH at nighttime, whereas the CMAQ

307   fire plume rise did not have these limitations.

308   **ASDTA**

309   The Automated Smoke Detection and Tracking Algorithm (ASDTA) is a combination of two data

310   sets: (1) the NOAA Geostationary satellite (G13) retrieves thermal enhancements aerosol optical depth

311   due to fires using visible channels and produces a product called GOES Aerosol/Smoke Product (GASP)

312   (Prados et al., 2007); and, (2) NOAA NESDIS HMS (Hazard Mapping System) fire smoke detection. First,

313   the observation of the increase in AOD near the fire is attributed to the specific HMS fire; AOD

314   values not associated with fires are dropped. Second, a pattern recognition scheme uses 30-

315   minutes geostationary satellite AOD images to tracks the transport of this smoke plume away

316   from the source. ASDTA provides the capability to determine whether the GASP is influenced by one or

317   multiple smoke plumes over a location at a certain time.

318   ASDTA is originally generate to provide operational support for verification of the NOAA HYSPLIT

319   dispersion model predicts smoke plume direction and extension (Draxler and Hess 1998). These data are

320   also suitable for model performance evaluation in this study. For each simulation, modeled AOD was

321   calculated for each sensitivity test ("with-fire" or "without-fire") and ΔAOD is defined as the difference

322   obtained by subtracting AOD_without-fire from AOD_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   Figure 7b presents similar results, but for simulated ΔAOD (with-fire – without-fire). For further

326   evaluation of the HMS detected smoke plume shape Fig. 7c can be compared with Figs. 7a and 7b.

327   Figure 7a shows several regions under the influence of fires in: California, northwest Mexico, Kansas,

328   Missouri, Oklahoma, Arkansas, Texas and part of the Gulf of Mexico. In the northeastern USA, fire

329   plumes occurred occasionally.   Those regions agreed relatively well with the shaded contours between

330   Figs. 7a and 7c. However, due to the lack of fire treatments in the CMAQ LBC, the simulation (Fig. 7b)

331   missed smoke influence on the northeast region of the CONUS domain. CMAQ also failed to simulate

332   the fire influences in the southwest region of the domain.

333   Similar plots for June 25 are shown in Figs. 7d, 7e and 7f for ASDTA, CMAQ and HMS,

334   respectively. The ASDTA (Fig. 7d) diagnosed an overestimation in fire influences in the south including

335   Texas and the Gulf of Mexico and an underestimation in the northeastern U.S. On the other hand, the

336   model predicted two strong fire signals clearly: near the border between Arizona and Mexico, and in

337   Colorado (See Fig. 7e). All the fire influenced areas in Fig. 7e were seen in observation by HMS in Fig. 7f.

338   Comparing ASDTA plots and CMAQ ΔAOD plots (Fig. 7a vs 7b; Fig. 7d vs 7e), both similarities and

339   differences were found. Similarities were attributable to similar fire accounting and meteorology.

340   Differences were attributable to: HMS contains more fire hotspots than those used by CMAQ due to

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341 domain size; only fires inside the CONUS were included in the CMAQ fire simulation and LBCs did not

342 vary to reproduce impacts of wildfires from outside of the domain.

SENEX

344   SENEX (Southeast Nexus) was a field campaign conducted by NOAA in cooperation with the US

345 EPA and the National Science Foundation in June and July 2013. Although SENEX was not specifically

346 designed for fire studies, its airborne measurements included $PM_{2.5}$ OC and EC, CO and acetonitrile

347 (CH_3CN). CH_3CN was chosen as a fire tracer since it is predominantly emitted from biomass burning

348 (Holzinger et al., 1999; Singh et al., 2012).

349   CH_3CN has a residence time in the atmosphere of around 6 months (Hamm and Warneck 1990)

350 and the reported CH_3CN background concentration is around 100 - 200 ppt (Singh et al., 2003).

351 Measured CH_3CN concentrations tend to increase with altitude (Singh et al., 2003; de Gouw et al., 2003),

352 since biomass burning plumes tend to ascend during long-range transport. During SENEX, measured

353 CH_3CN showed a similar pattern. Fire signals were identified through airborne measurements of CH_3CN

354 when its concentration exceeded the background; e.g., on July 3 2013, or when its concentration peak

355 appeared at high altitude; e.g., on June 16 2013 and July 10 2013.

356   CH_3CN airborne measurements were used to identify fire plumes at certain locations and

357 heights during SENEX. For model evaluations, fire locations and accurate meteorological wind field are

358 crucial to interpret 2-D measurements such as IMPROVE, HMS and ASDTA. To verify a 3-D fire field, it is

359 critical to capture plume rise. However, it was extremely difficult to back out plume rise from the

360 airborne measurements. An additional uncertainty arose in the difference of temporal resolutions of the

361 data: IMPROVE, HMS shapefiles and ASDTA were daily or hourly data, whereas airborne CH_3CN data

362 were measured at one-minute intervals.

363   Figure 8a shows a CMAQ simulated ΔCO vertical distribution along flight transects on June 16

364   2013. This flight occurred during the weekend over and around power plants around Atlanta, GA. The

365   color of flight path represents observed CH_3CN concentration in ppt. In Fig. 8a, the concentration of ΔCO

366   increased from surface to 5000 m, especially above 2000 m. Six CH_3CN concentration peaks were

367   observed when AGL was above 2500 m.

368   For CMAQ simulated ΔCO, five out of six fire signals detected by CH_3CN measured spikes were

369   captured where ΔCO concentrations were all above 3 ppb. Only one fire signal was missed by the model

370   at 18:30 UTC June 16 2013. Model simulation showed that long range transports (LRT) of smoke plumes

371   influenced airborne observations. Fire signals from the free troposphere subsided and influenced flight

372   measurements. High EC or OC or CO did not concur with high CH_3CN observation probably due to

373   species lifetime differences. HMS smoke plume did not show any hotspots or smoke plume around

374   Atlanta suggesting that the sources of those observed fire signals were not from its vicinity.

375   A similar phenomenon was seen in SENEX flight 0710, which occurred during flight transects

376   from Tennessee to Tampa, FL. Figure 8b is a similar graph as Fig. 8a. Based on ΔCO concentrations,

377   CMAQ captured the July 10 case as fire signals were observed. Nonetheless, ΔCO may be over predicted

378   at around 19 UTC. The model exhibited a fire signal with ΔCO concentration of about 3 ppb near 6000 m

379   around 19 UTC, whereas measured CH_3CN was 120 ppt.

380   **SENEX flight on July 3**

381   Observations from IMPROVE, HMS and SENEX identified fire signals on July 3 2013. ASDTA

382   retrievals were not available. Those signals were missed by the model. In this section, all of evaluation

383   methods addressed above were used to study potential causes of failure of the model to reproduce fire

384   signals.

385   At the MACA IMPROVE site on July 3 2013, the wind direction at the surface was southeasterly,

386   with no fire hotspots (solid black circle) located upwind of MACA (Fig. 9a). Without any identified

387   hotspots upwind, the model missed fire signals observed at MACA on July 3 2013.

388   Flight #0703 was a night mission targeting power plants in Missouri and Arkansas. The flight

389   path is shown in Fig. 9b and is colored by measured CH_3CN concentration. In order to highlight CH_3CH

390   concentrations above 400 ppt in the measurements, CH_3CN concentrations below 400 ppt were

391   represented by black dots. During the flight, 16 measurements of acetonitrile concentration above 400

392   ppt were observed and the maximum was 3227.9 ppt. These observations were located over

393   northwestern Tennessee and close to the borders of Kentucky, Illinois, Missouri and Arkansas. Except

394   for one observation, the flight ASL was between 500 m and 1000 m.

395   Enhancements of CO and OC were also measured concurrently with CH_3CN. Figures 9c and 9d

396   show scatter plots for CH_3CN versus CO and OC, respectively. Measured CH_3CN was highly correlated to

397   both measured CO and OC, with linear correlation coefficients (R^2) of 0.83 and 0.71, respectively. The

398    $\Delta CH_3CN/\Delta CO$ ratio is around 2.7 (ppt/ppb), which is consistent with findings of other measurements

399   over California in 2002 when a strong forest fire signal was intercepted by aircraft (de Gouw et al.,

400   2003). The $\Delta CH_3CN/\Delta OC$ ratio was around 6.85 (ppt/(mg m^{-3})), which is also in the range of biomass

401   burning analyses in MILAGRO (Megacity Initiative Local and Global Research Observations) (Aiken et al.,

402   2010).

403   Figure 9e shows model simulated ΔCO with peaks at AGL below 3000 m. Fire signals showed

404   substantial influences on aircraft measurement at around 5 UTC. However, clear fire signals between 2

405   UTC and 3 UTC were observed based on prior CH_3CN analysis. The model either predicted insufficient

406   fire emission influences or missed it. FMS score on July 3 was 30%. Figure 9f shows that CMAQ did not

407   predict plumes where the HMS plume analysis exhibited several dense smoke plumes. As NOAA Smoke

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408   Text Product (http://www.ssd.noaa.gov/PS/FIRE/DATA/SMOKE) described on its July 03 0501 UTC

409   report: a smaller very dense patch of remnant smoke, analyzed earlier the same day over southern

410   Missouri, drifted southward into Arkansas."

411   The reasons the model missed these fire observations were not clear. Figures 10, 11a and 11b

412   suggest a few clues. Figure 10 is a backward trajectory analysis plot for the observations obtained during

413   the SENEX flight on July 3 with CH_3CN measured concentration above 400 ppt. Both transect and passing

414   altitude of the air parcels clearly showed those measurements were most likely influenced by the nearby

415   pollution sources. Figure 11a illustrates the locations of fire used in the CMAQ simulation. It is noted

416   that hmshysplit.txt is input into BlueSky after HMS quality control (Fig. 1). There were several hotspots

417   around the region where the IMPROVE site MACA was located and where the SENEX flight overpassed.

418   Our fire simulation system might have underestimated smoke emissions from those fires. Other

419   explanation was from Fig. 11b, which illustrated hotspots in hmx.txt. In hmx.txt, every detected fire

420   spots by HMS before quality control were showed. Comparing Fig. 11a with 11b, there were clusters of

421   fire spots in the central U. S. especially in West Tennessee. However, those spots were removed during

422   the HMS quality control process because there were no associated smoke plumes visible. In most of

423   times, those fires were believed to be small sized fires such as from agriculture fires or prescribed burns.

424   For this case, there seem to have been thin clouds overhead and thicker clouds in the vicinity,

425   (http://inventory.ssec.wisc.edu/inventory/image.php?sat=GOES-13&date=2013-07

426   03&time=16:02&type=Imager&band=1&thefilename=goes13.2013.184.160147.INDX&coverage=CONUS

427   &count=1&offsettz=0), so it would be hard to differentiate smoke from clouds by satellite observations

CONCLUSIONS

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429   In support of the NOAA SENEX field experiment in June-July 2013, simulations were conducted

430   including smoke emissions from fires. In this study, a system accounting for fire emissions in a chemical

431   transport model is described, including a satellite fire detecting system (HMS), a fire emission calculation

432   model (BlueSky), a pre-processing of fire emissions (SMOKE), and simulation over the SENEX domain by

433   CMAQ. The focus of this work is to evaluate the system's capability to capture fire signals identified by

434   multiple observation data sets. These data sets included IMPROVE ground station observations, satellite

435   observations (HMS plume shapefile and ASDTA) and airborne measurements from the SENEX campaign.

436   For IMPROVE data, potential fire signals were identified by measured potassium concentrations

437   in $PM_{2.5}$. Fire identifications in CMAQ rely on predicted ΔCO, the difference between simulations with

438   and without fire emissions. Three out of four observed fire signals were captured by CMAQ simulations.

439   For HMS smoke plume shapefiles that were manually plotted by analysts to represent the regions

440   impacted by smoke, we used FMS to calculate the percentage of its overlapping with CMAQ predicted

441   smoke plumes. FMS averaged 22% over forty days of the SENEX campaign. In terms of fire smoke

442   impacts on ΔAOD, both ASDTA and CMAQ showed patterns that were compared to HMS plume

443   shapefile. In terms of measured CH_3CN, a biomass burning plume tracer, both SENEX aircraft in-flight

444   measurements and CMAQ simulations captured signatures of long range transport of fire emissions

445   from elsewhere in the CONUS domain.

446   Generally, using HMS-detected fire hotspots and smoke data was useful for predictions of fire

447   impacts and their evaluation. The HMS-BlueSky-SMOKE-CMAQ fire simulation system, which is also used

448   in NAQFC, was able to capture most of the fire signals detected by multiple observations. However, the

449   system failed to identify fire cases on June 17 and July 3 2013 -- thereby demonstrating two problems

450   with the simulation system. One identified problem was the lack of a dynamical fire LBC bounding the

451 CONUS domain to represent the inflows of strong fire signals originating from outside the simulation

452 domain. Secondly, the HMS quality control procedure eliminated fire hotspots that were not associated

453 with visible smoke plumes leading to an underestimation.

454   We were keen on understanding and quantifying the various uncertainties and observational

455 constraints of this study therefore the following rules of thumb were observed: (1) a holistic evaluation

456 approach was adopted so that the fire smoke algorithm was interpreted as a single entity to avoid

457 deadlock due to over-interpretation of uncertainty of the single component in the system; (2) analysis

458 conclusion applicable to the entire simulation period was drawn so that the episodic characteristics of

459 the cases embedded in the simulation were averaged and generalized. This new methodology may

460 benefit NAQFC; (3) we took advantage of the multiple perspectives of the observation systems that

461 offered a wide spectrum of temporal and spatial variabilities intrinsic to the systems; (4) we were

462 intentionally conservative in discarding data so that we maximized the sampling pool for statistical

463 analysis and avoided unwittingly discarding poorly simulated cases, good outliers, and weak but

464 accurate signals.

465   Quantitative evaluation of fire emissions and their subsequent influences on ozone and

466 particulate matter in this fire and smoke prediction system is challenging. Future work includes applying

467 these findings to the NAQFC and improving the NAQFC system's capabilities to simulate fires accurately.

Code Availability

469   The source code used in this study is available online at

470 http://www.nco.ncep.noaa.gov/pmb/codes/nwprod/cmaq.v5.0.2.

Acknowledgements & disclaimer

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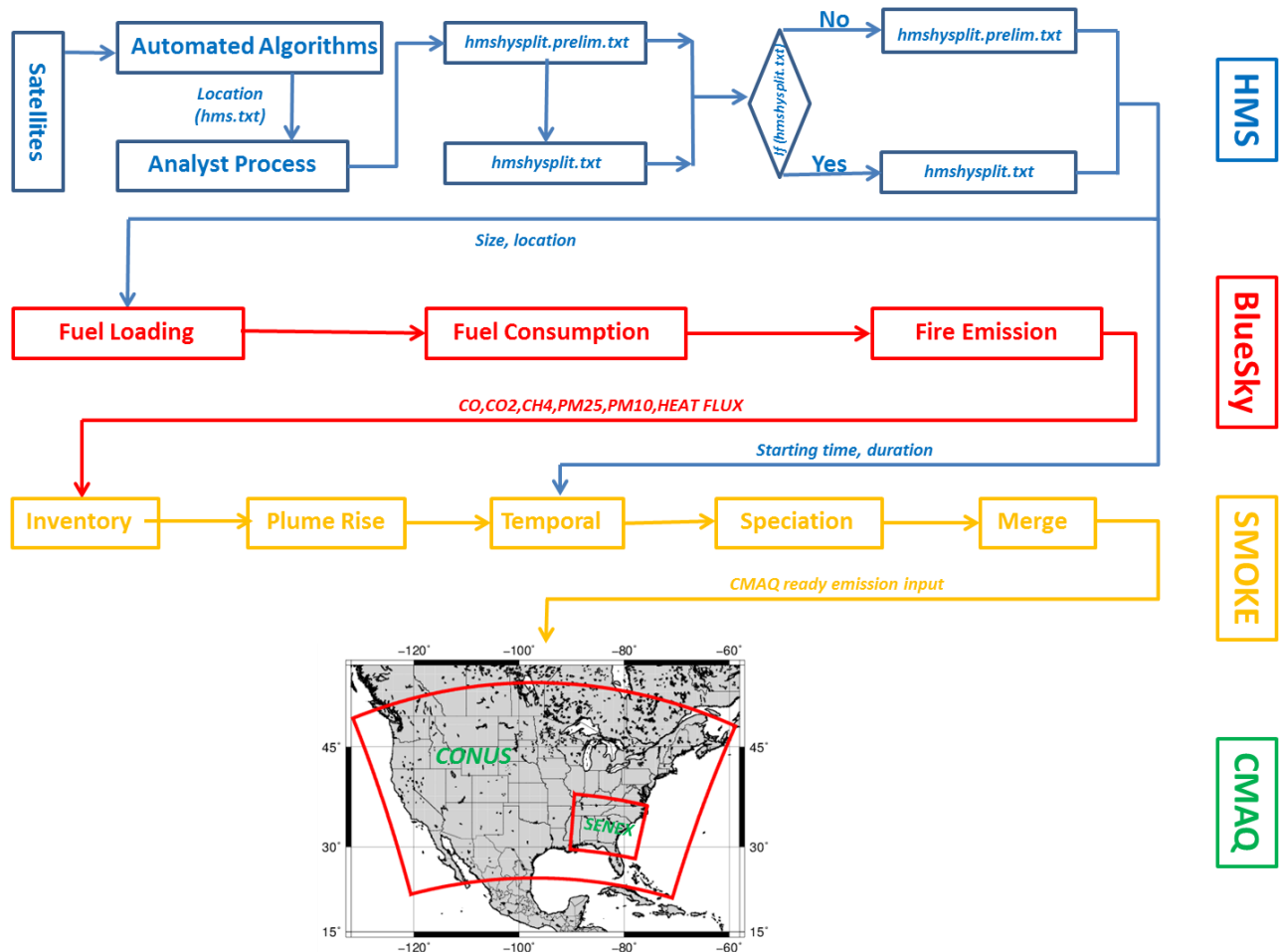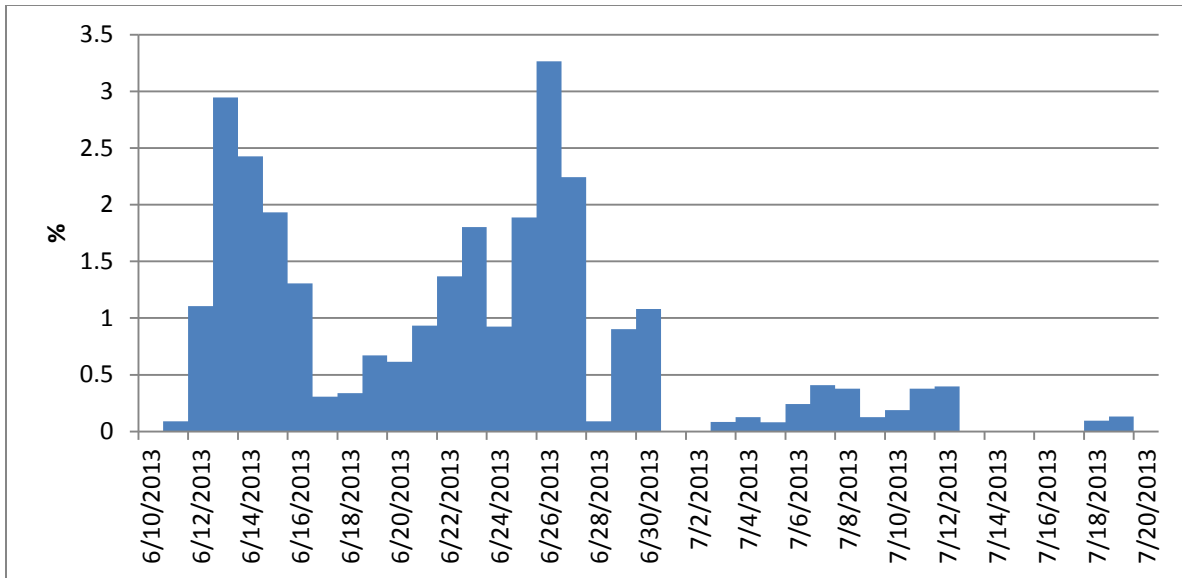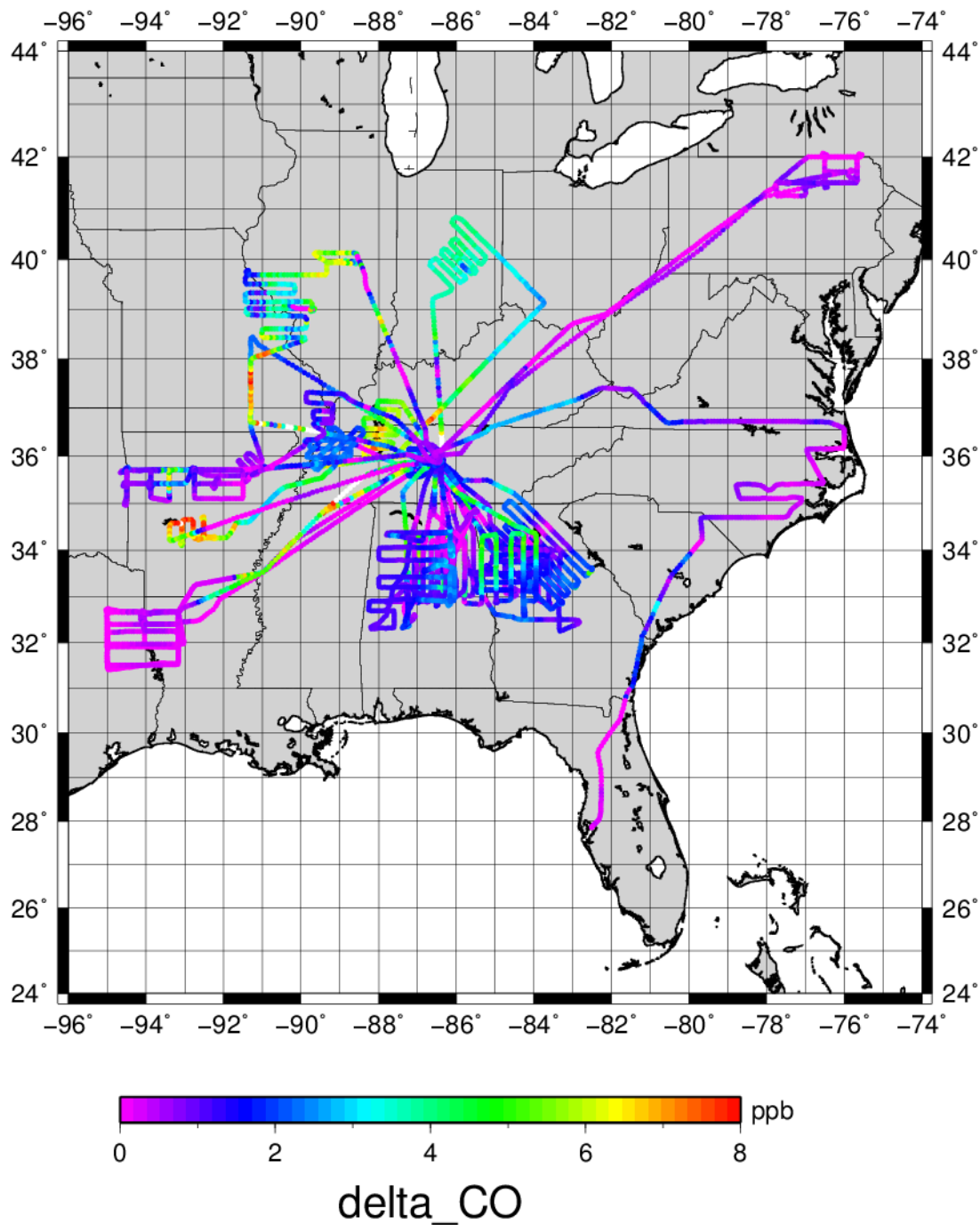482

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Figures:

Figure 1, schematics of fire emission and smoke plume simulation system used: Data-feed and/or modeling of physical and chemical processes were handled largely sequentially from top to bottom and from left to right; The right hand four vertical boxes depict the submodel names: NESDIS Hazard Mapping System (HMS) for wild fire hot spot detection; US Forest Service's BlueSky for fuel type and loading parameterization; and US EPA's Sparse Matrix Operator Kernel (SMOKE) to handle emission characterization; and lastly the Community Multiple-scale Air Quality model (CMAQ) was applied to simulate the transformation, transport and depositions of the atmospheric constituents. The "SENEX" in-set framed by red emboldened lines was the domain for this study.
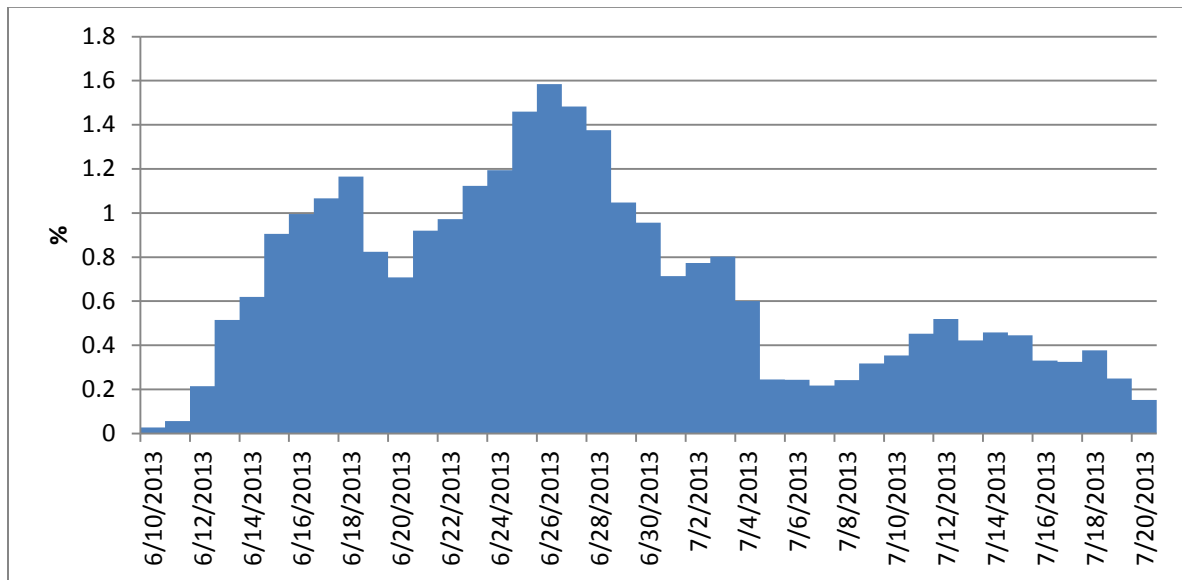
Figure 2, in 4km SENEX domain, (a): the contribution (%) of CO emission from fires occurred inside the SENEX domain; (b): the contribution (%) of CO flux flowing into the SENEX domain from its boundary caused by fires burning outside the SENEX domain but inside the CONUS domain.

Figure 3, CMAQ simulated ΔCO (ppb): i.e., the CO concentration difference between CMAQ simulation with and without fire emissions, extracted along the overall SENEX flight paths during the SENEX campaign between June 10 and July 20 2013.

Figure 4, simulated ΔCO (>2.0 ppb) in the SENEX domain on June 24 2013 at 20:00 UTC overlaid with 2 m wind arrows with a 10 m s^{-1} reference arrow shown in the bottom right. The solid black circle is detected fire hotspots by HMS. The solid triangles labeled with station code represents IMPROVE sites used in model verification calculations.

Figure 5, FMS (Figure of Merits in Space) (%) from June 11 to July 19 in 2013 during the SENEX campaign.

Figure 6, Daily HMS observed plume shape versus CMAQ predicted daily averaged plume shape on (a): July 6 2013; (b): June 17 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. (c): HMS observed fire hotspots (red) and plume shapes (white) (http://ready.arl.noaa.gov/data/archives/fires/national/arcweb) on June 17, 2013.

Figures 7, GOES detected AOD influenced by fires using ASDTA diagnose method (summed over from 10:00 am to 2:00 pm local time). Color-shaded region represents the fire-smoke influenced areas and the color denotes the magnitude of the retrieved AOD on (a): June 14 2013; (d): June 25 2013; simulated ΔAOD (withfire – nofire) calculated by CMAQ on (b): June 14 2013; (e): June 25 2013; HMS observed fire hotspots (red) and plume shapes (white) on (c): June 14 2013; (f): June 25 2013.

Figure 8, vertical distributions of CMAQ simulated ΔCO (ppb) shown along flight transect on (a): June 16 2013; (b): July 10 2013; the x-axis label is UTC (hour) and y-axis label is AGL (m). Two color bars represent observed CH3CN concentration (filled square dots and rectangle bar in ppt) and simulated ΔCO concentration (backdrop color shading and fan bar in ppb), respectively.

Figure 9, plots for July 3 2013 case, (a): IMPROVE; (b): the flight path of SENEX #0703 colored by measured CH$_3$CN concentration (ppt); (c): CH$_3$CN (ppt) vs CO (ppb); (d): CH$_3$CN (ppt) vs AMS_Org (mg m$^-$

526   ^{3}); (e): CMAQ simulated ΔCO vertical distributions along flight transect; (f): HMS observed plume shape

527   versus CMAQ prediction.

528   Figure 10, a backward trajectory analysis for CH_3CN concentration in ppt greater than 400 ppt measured

529   along a SENEX flight on July 03 in: (upper) aerial, and (lower) time vertical cross-sections.

530   Figure 11, detected fire hotspots on July 03 2013 as daily composite (a): hmxhysplit.txt; (b): hmx.txt.

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Satellites → Automated Algorithms

Location (hms.txt)

Analyst Process

hmshysplit.prelim.txt

hmshysplit.txt

If (hmshysplit.txt)

No → hmshysplit.prelim.txt

Yes → hmshysplit.txt

HMS

Size, location

Fuel Loading → Fuel Consumption → Fire Emission

BlueSky

CO,CO2,CH4,PM25,PM10,HEAT FLUX

Starting time, duration

Inventory → Plume Rise → Temporal → Speciation → Merge

SMOKE

CMAQ ready emission input

−120° −100° −80° −60°

45° CONUS 45°

30° SENEX 30°

15° 15°

−120° −100° −80° −60°

CMAQ

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Figure 1: schematics of fire emission and smoke plume simulation system used: Data-feed and/or modeling of physical and chemical processes were handled largely sequentially from top to bottom and from left to right; The right hand four vertical boxes depict the submodel names: NESDIS Hazard Mapping System (HMS) for wild fire hot spot detection; US Forest Service's BlueSky for fuel type and loading parameterization; and US EPA's Sparse Matrix Operator Kernel (SMOKE) to handle emission characterization; and lastly the Community Multiple-scale Air Quality model (CMAQ) was applied to simulate the transformation, transport and depositions of the atmospheric constituents. The "SENEX" in-set framed by red emboldened lines was the domain for this study.

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

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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.

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Figure 3: CMAQ simulated ΔCO (ppb): i.e., the CO concentration difference between CMAQ simulation with and without fire emissions, extracted along the overall SENEX flight paths during the SENEX campaign between June 10 and July 20 2013.

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Figure 5: FMS (Figure of Merits in Space) (%) from June 11 to July 19 in 2013 during the SENEX campaign.

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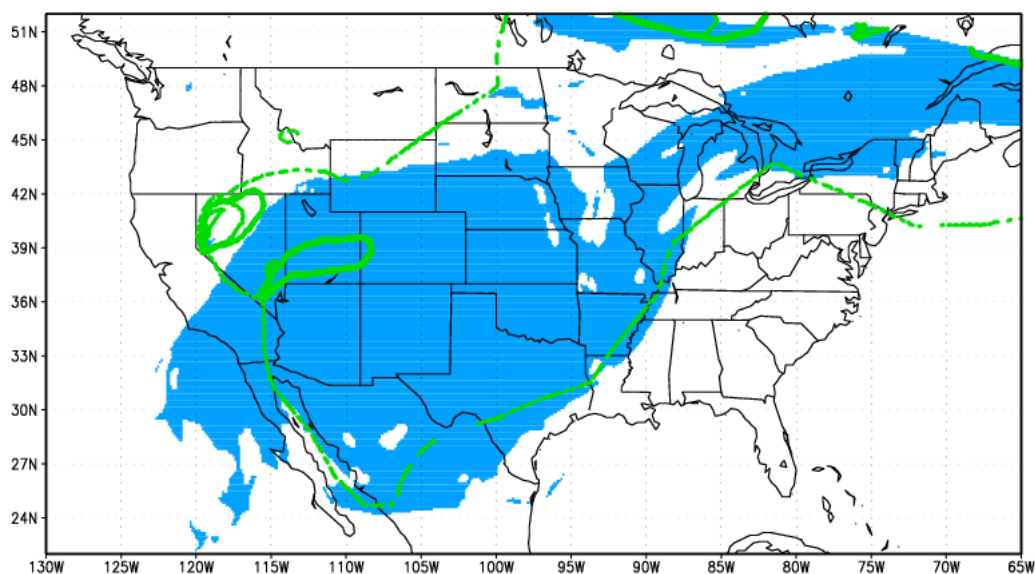
Figure 6a: Daily HMS observed plume shape versus CMAQ predicted daily averaged plume shape on July 6 2013; The light blue shading represents modeled plume shape (defined as total column ΔCO) and the thin dash line and emboldened green lines encircle areas representing HMS-derived light and strong influenced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

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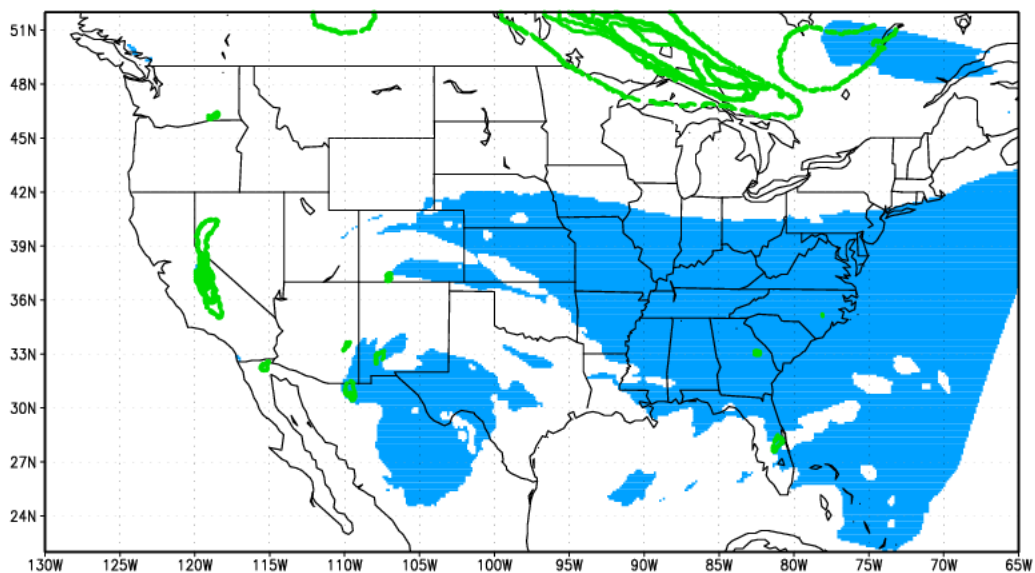
Figure 6b: same as Figure 6a but for June 17 2013.

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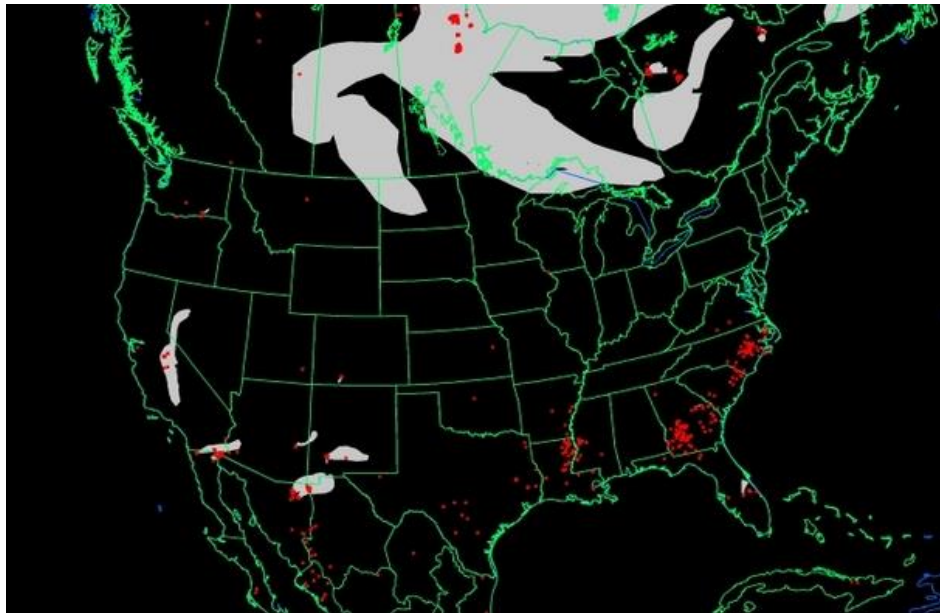
Figure 6c: HMS detected fire hotspots (red) and smoke plume shapes (white) on June 17 2013
(analysis day: 20130717, map generated: around 1100 GMT).
(http://ready.arl.noaa.gov/data/archives/fires/national/arcweb).

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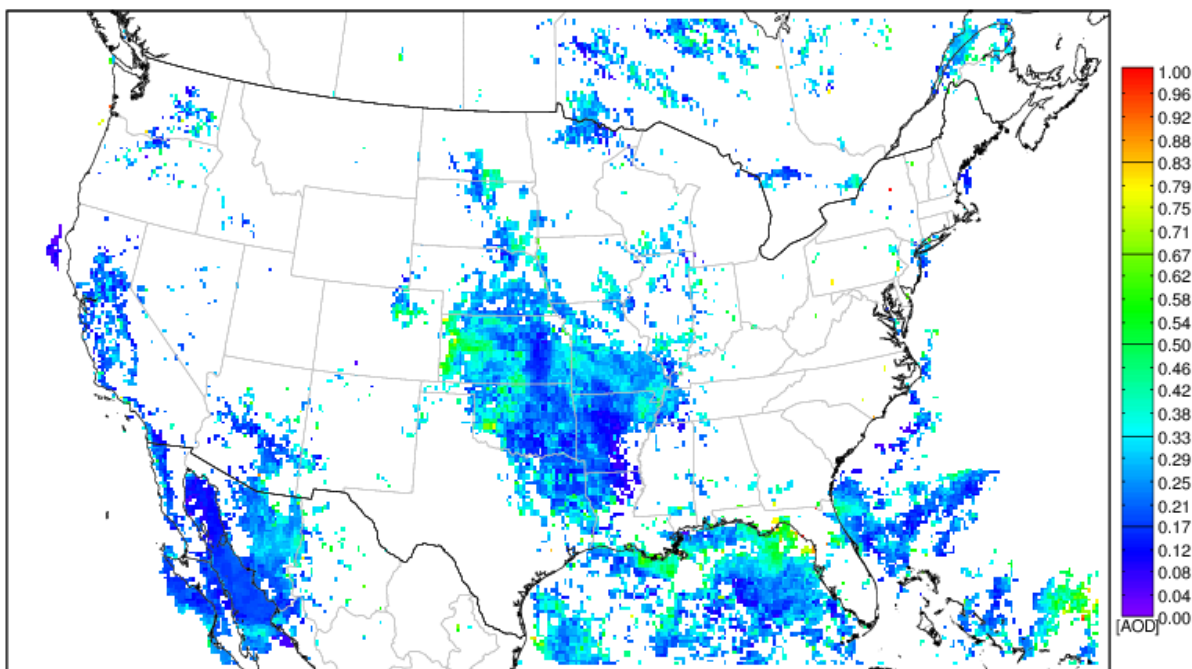
Figure 7a: GOES detected AOD influenced by fires using ASDTA diagnose method on June 14 2013

(summed over from 10:00 am to 2:00 pm local time). Color-shaded region represents the fire-smoke

influenced areas and the color denotes the magnitude of the retrieved AOD.

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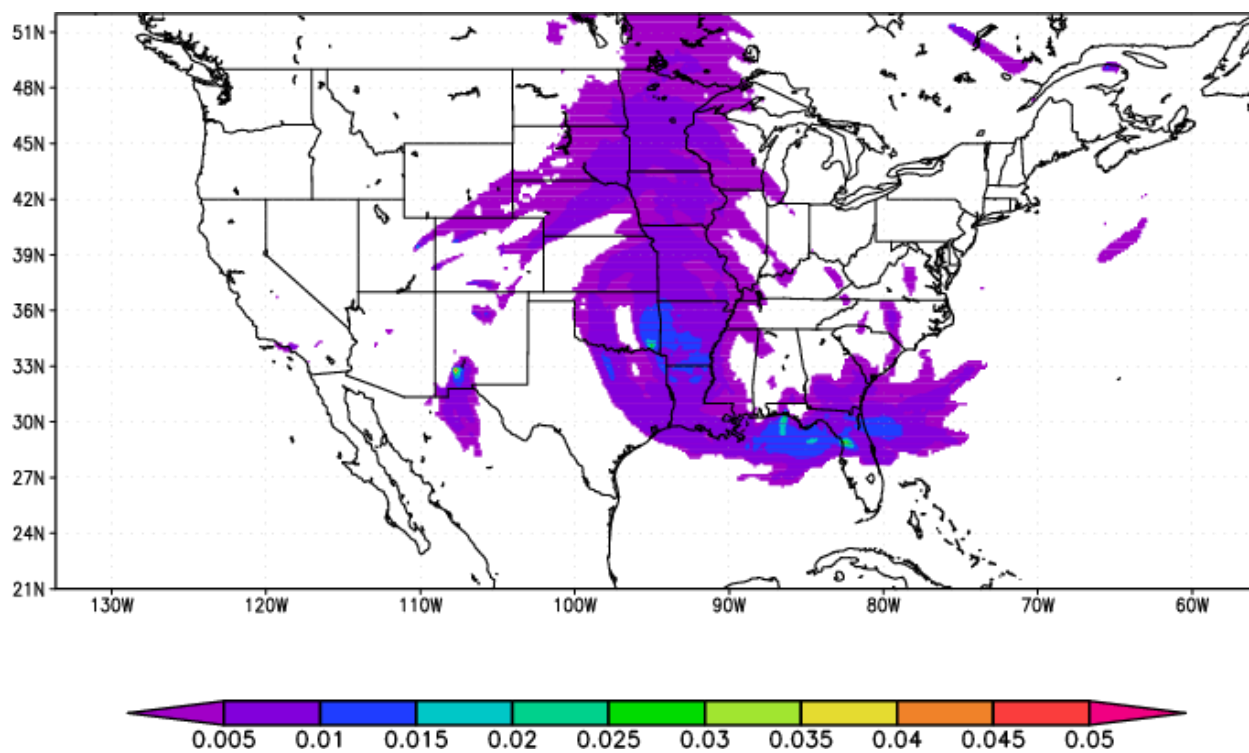
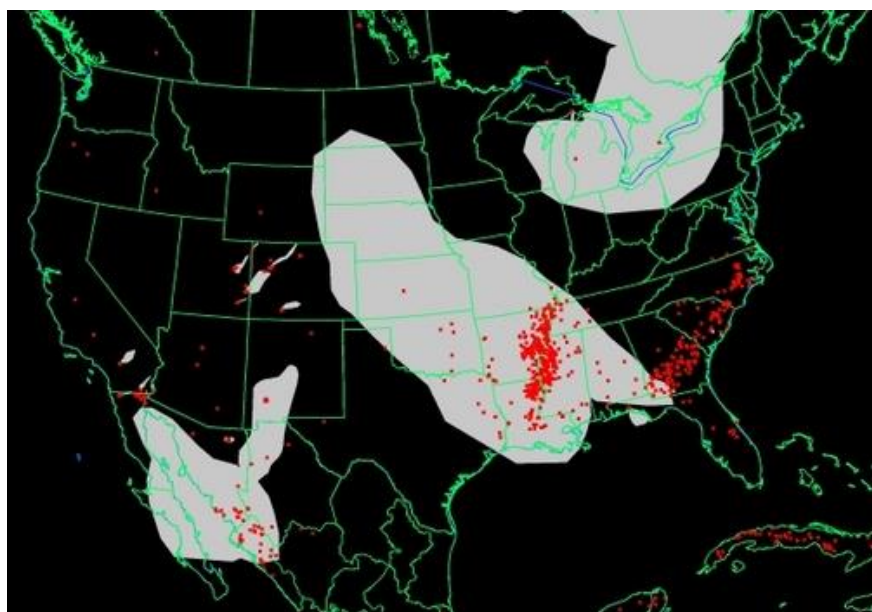**Figure 7b: simulated ΔAOD (with-fire – without-fire) calculated in CMAQ on June 14 2013.**

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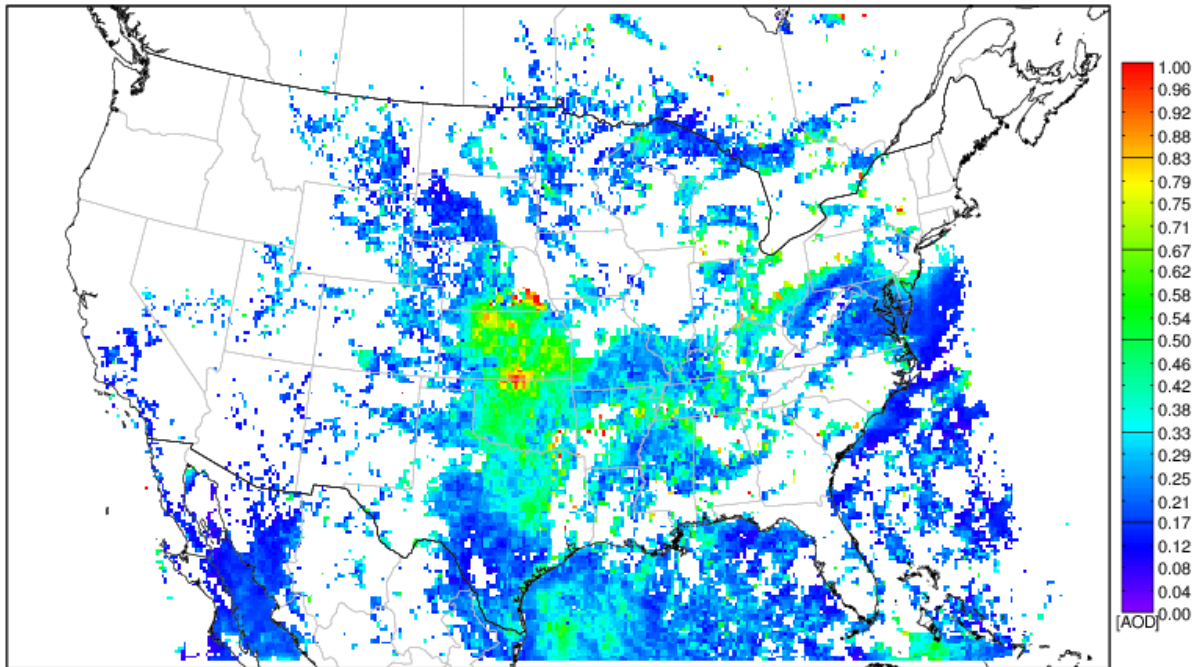609   **Figure 7c: same as Figure 6c but for June 14 2013.**

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Figure 7d: same as Figure 7a but for June 25 2013.
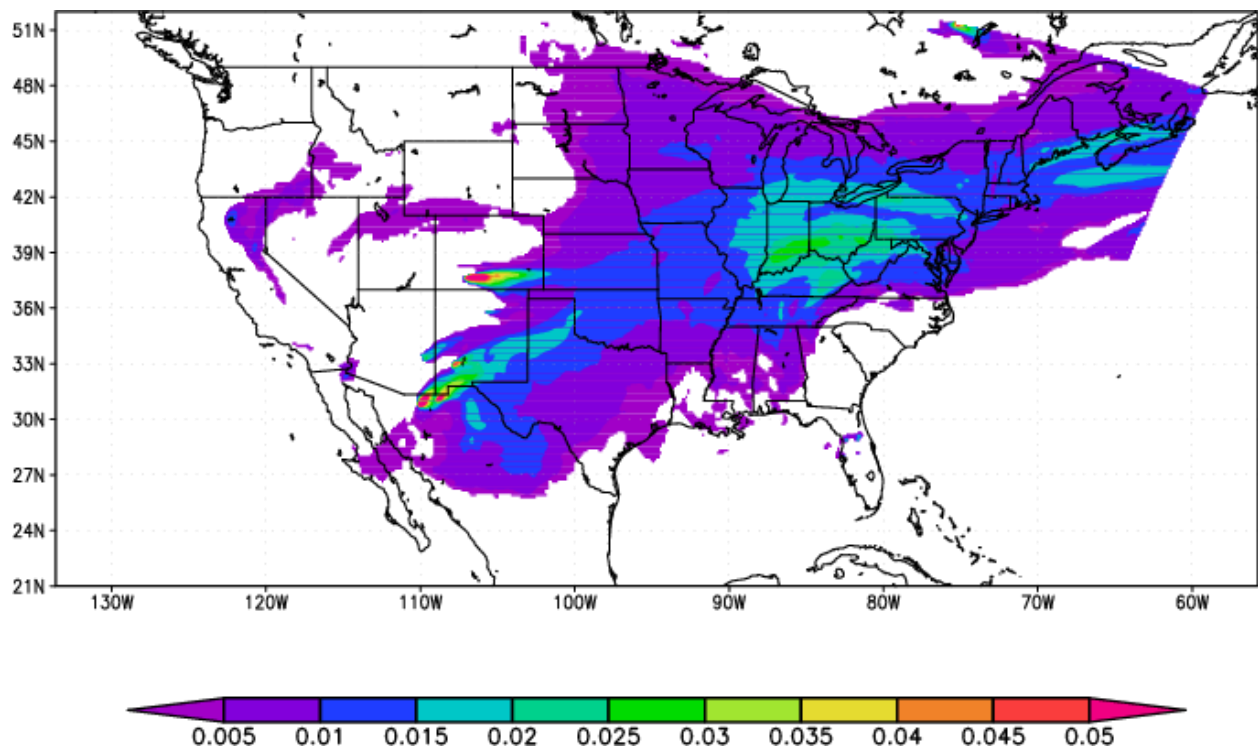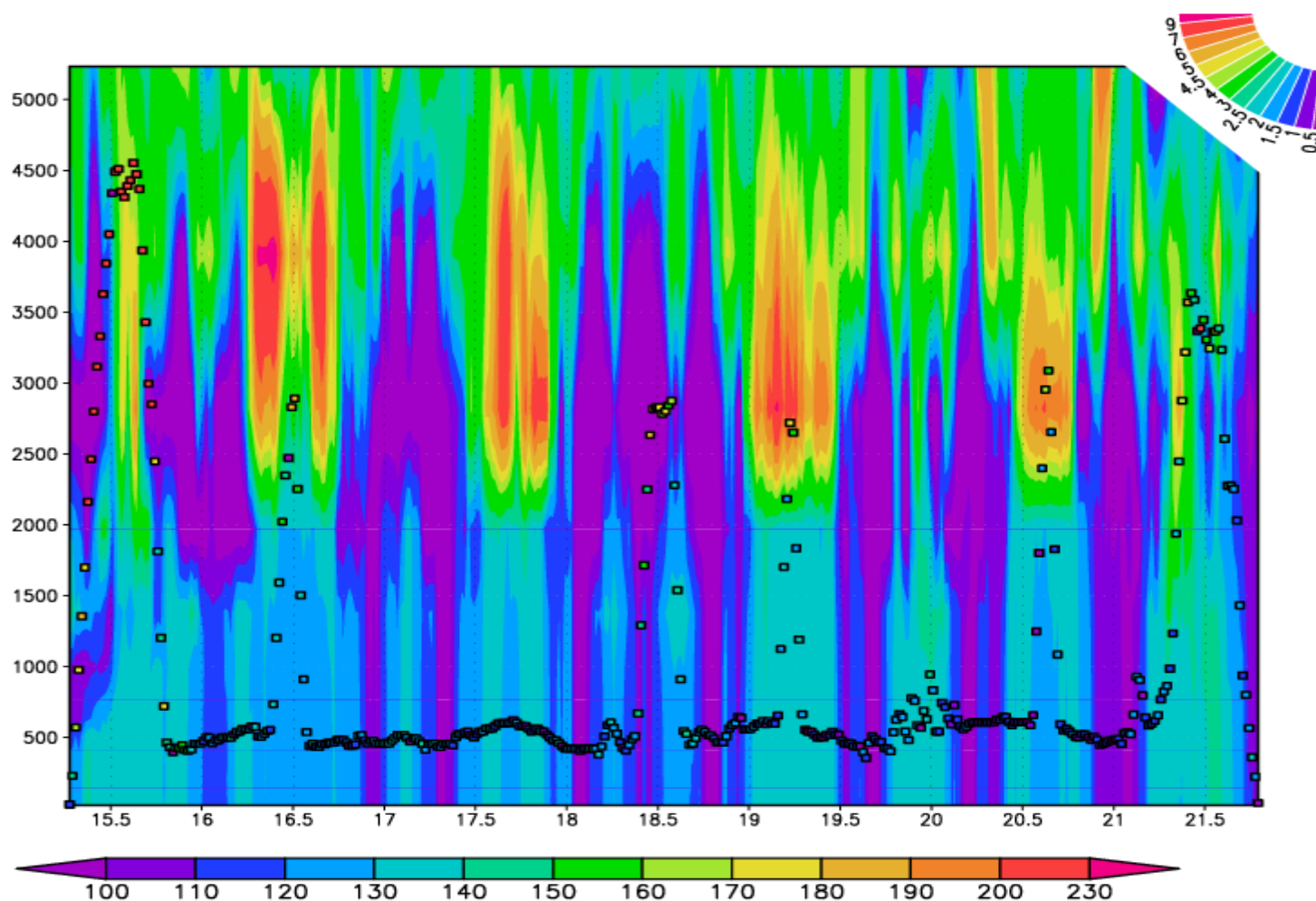
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Figure 7e: same as Figure 7b but for June 25 2013.

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618   **Figure 7f: same as Figure 6c but for June 25 2013.**

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Figure 8a: vertical distributions of CMAQ simulated ΔCO (ppb) shown along flight transect on June 16 2013. The x-axis label is UTC (hour) and y-axis label is AGL (m). Two color bars represent observed CH_3CN concentration (filled square dots and rectangle bar in ppt) and simulated ΔCO concentration (backdrop color shading and fan bar in ppb), respectively.
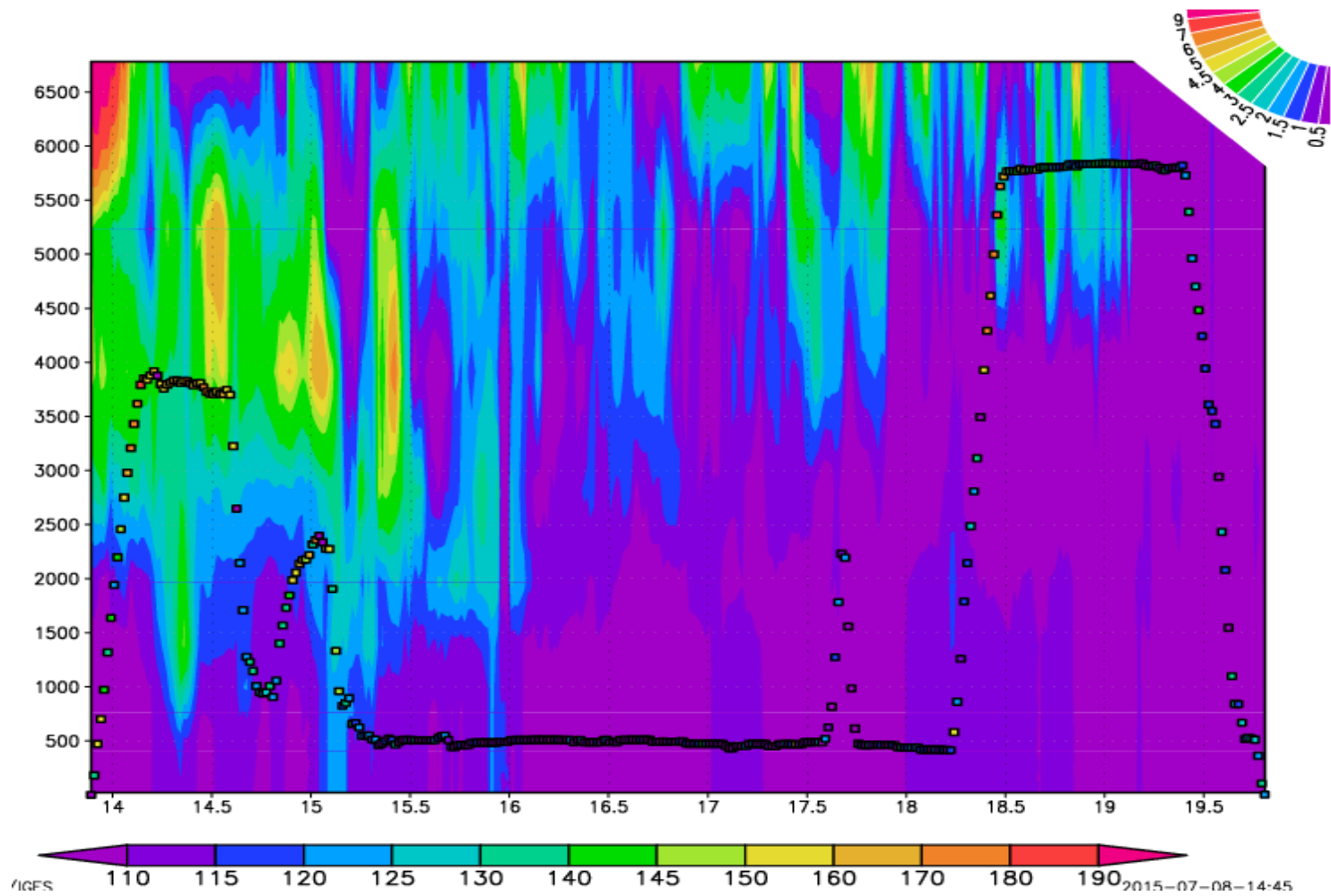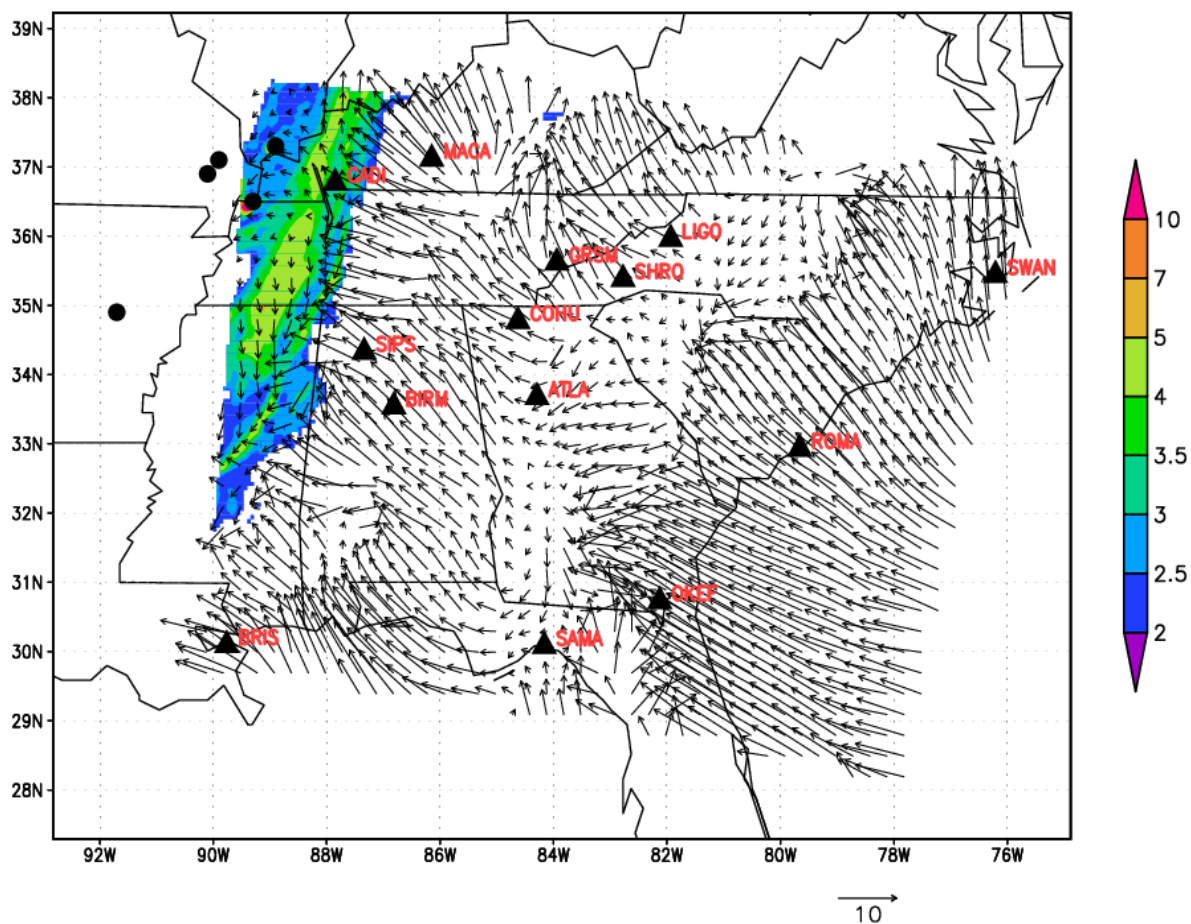
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627 **Figure 8b: same as Figure 8a but for July 10 2013.**
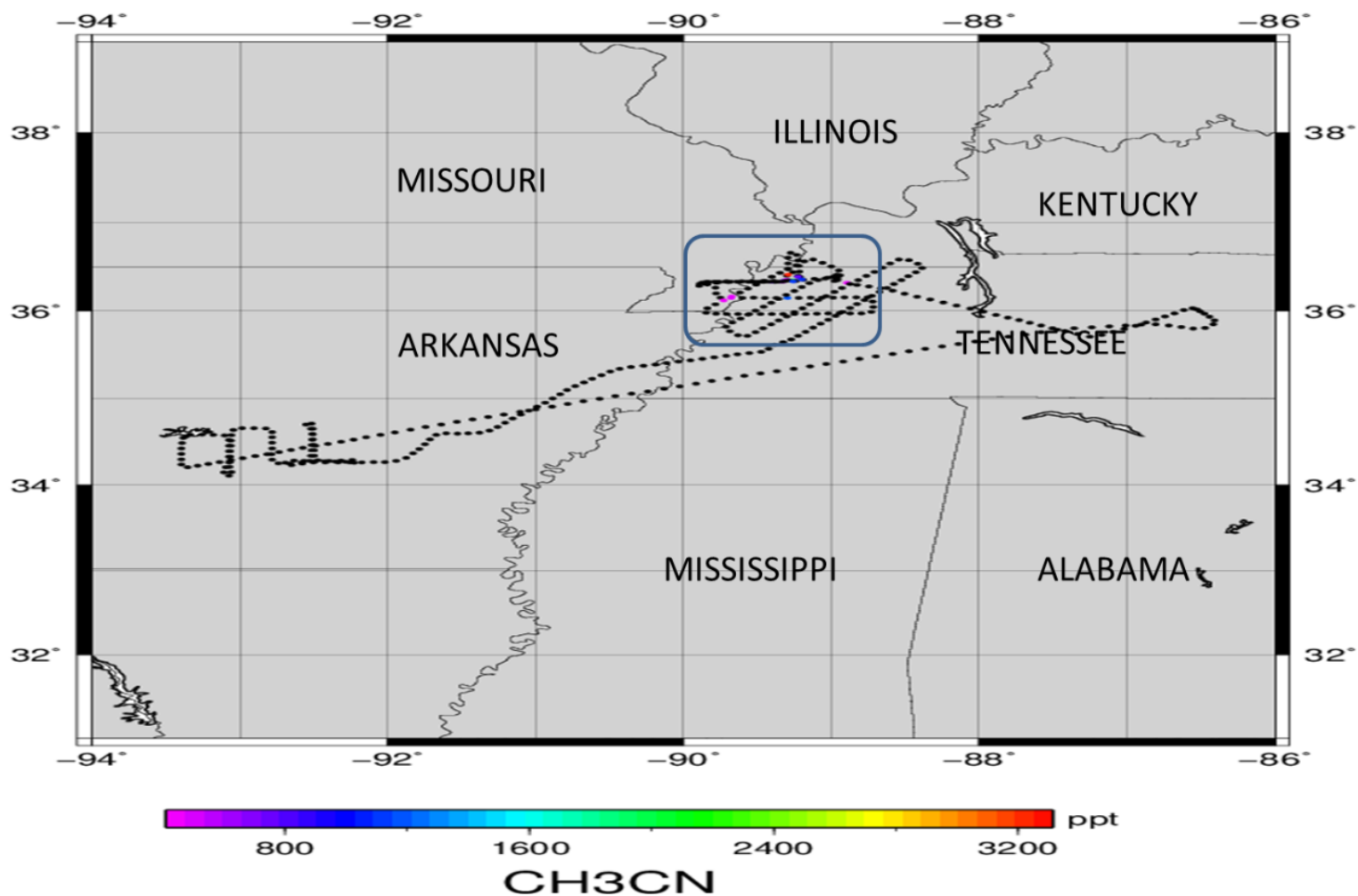
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Figure 9a: same as Figure 4 but for July 03 2013.

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Figure 9b: the flight path of SENEX #0703 traversed the Central Plain between local time 10:00pm and 11:00pm on July 02, 2013 --- colored by measured CH3CN concentration (ppt).

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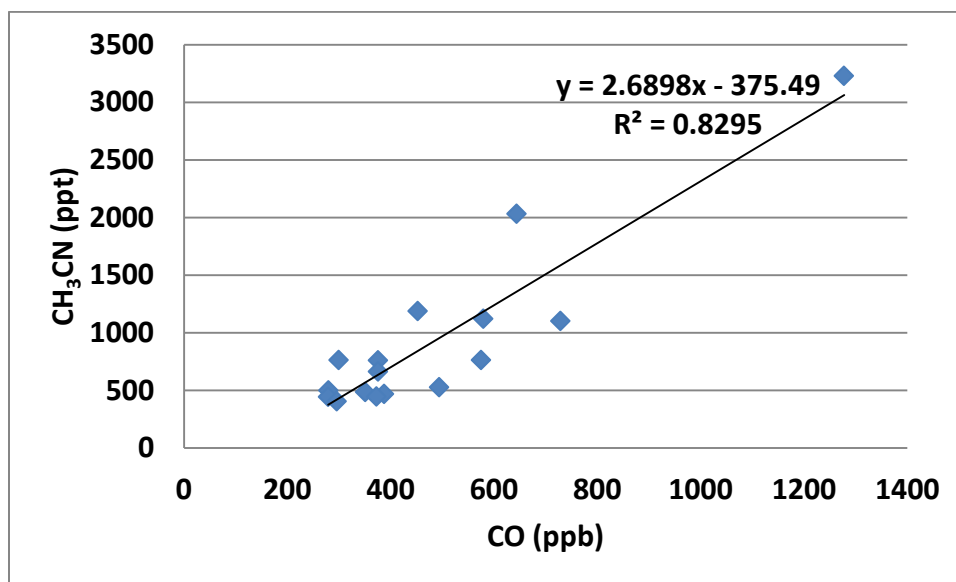
Figure 9c: CH$_3$CN (ppt) vs CO (ppb) scatter plot.
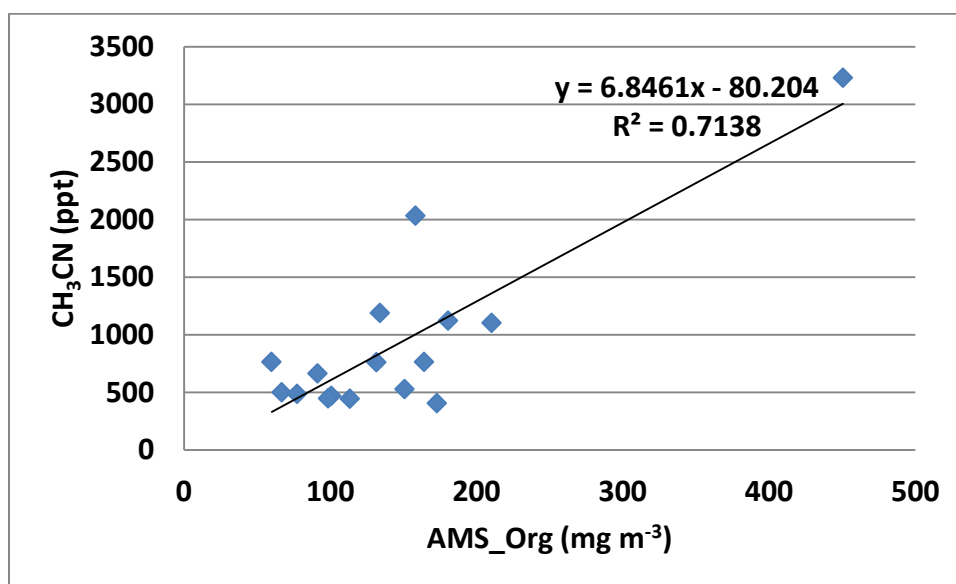
Figure 9d: CH$_3$CN (ppt) vs AMS_Org (mg m^{-3}) scatter plot.

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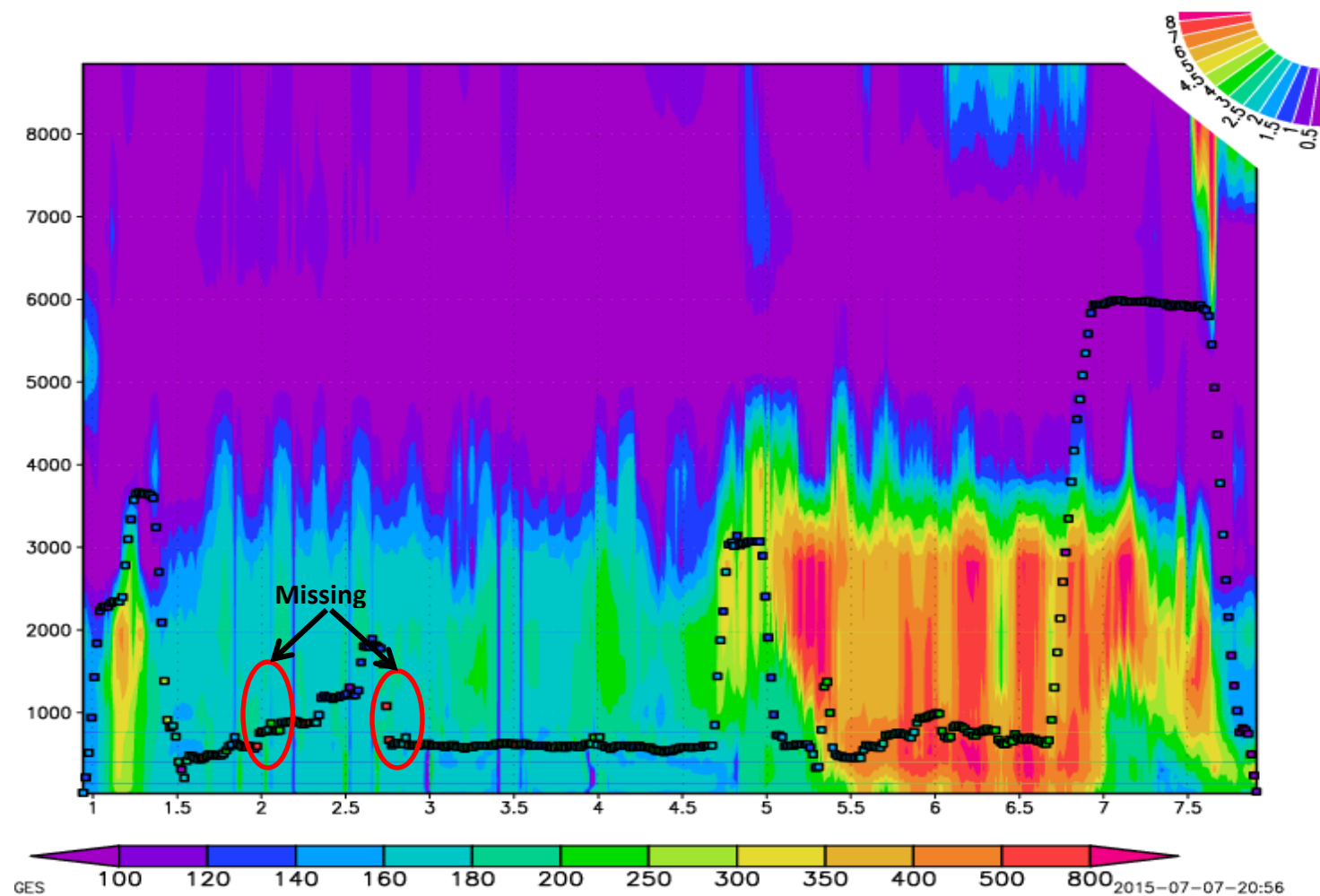
Figure 9e: same as Figure 8a but for July 03 2013. The emboldened red ovals highlighted missing CH$_3$CN concentration measurements.

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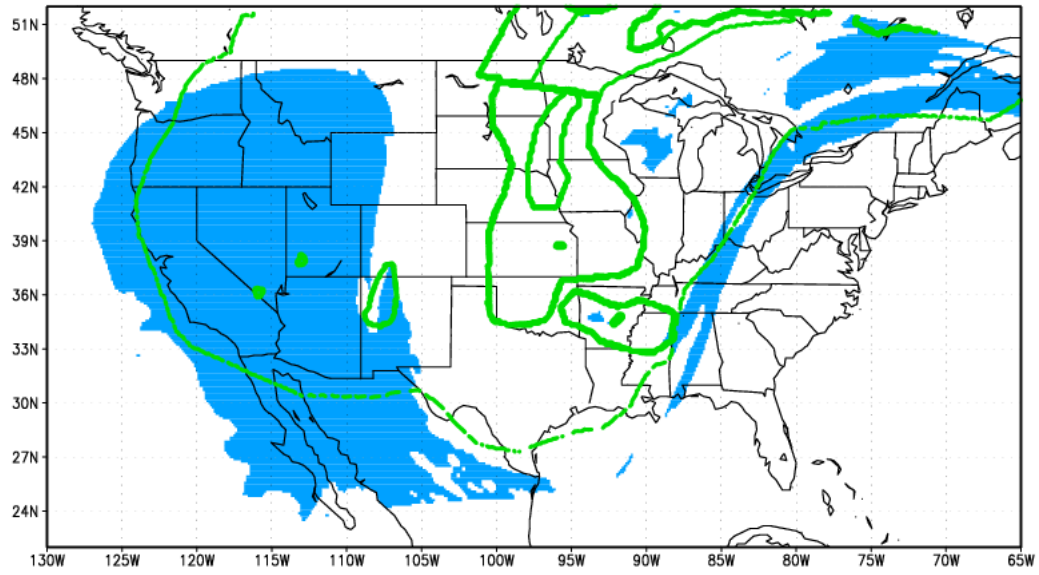
Figure 9f: same as Figure 6a but for July 03 2013.
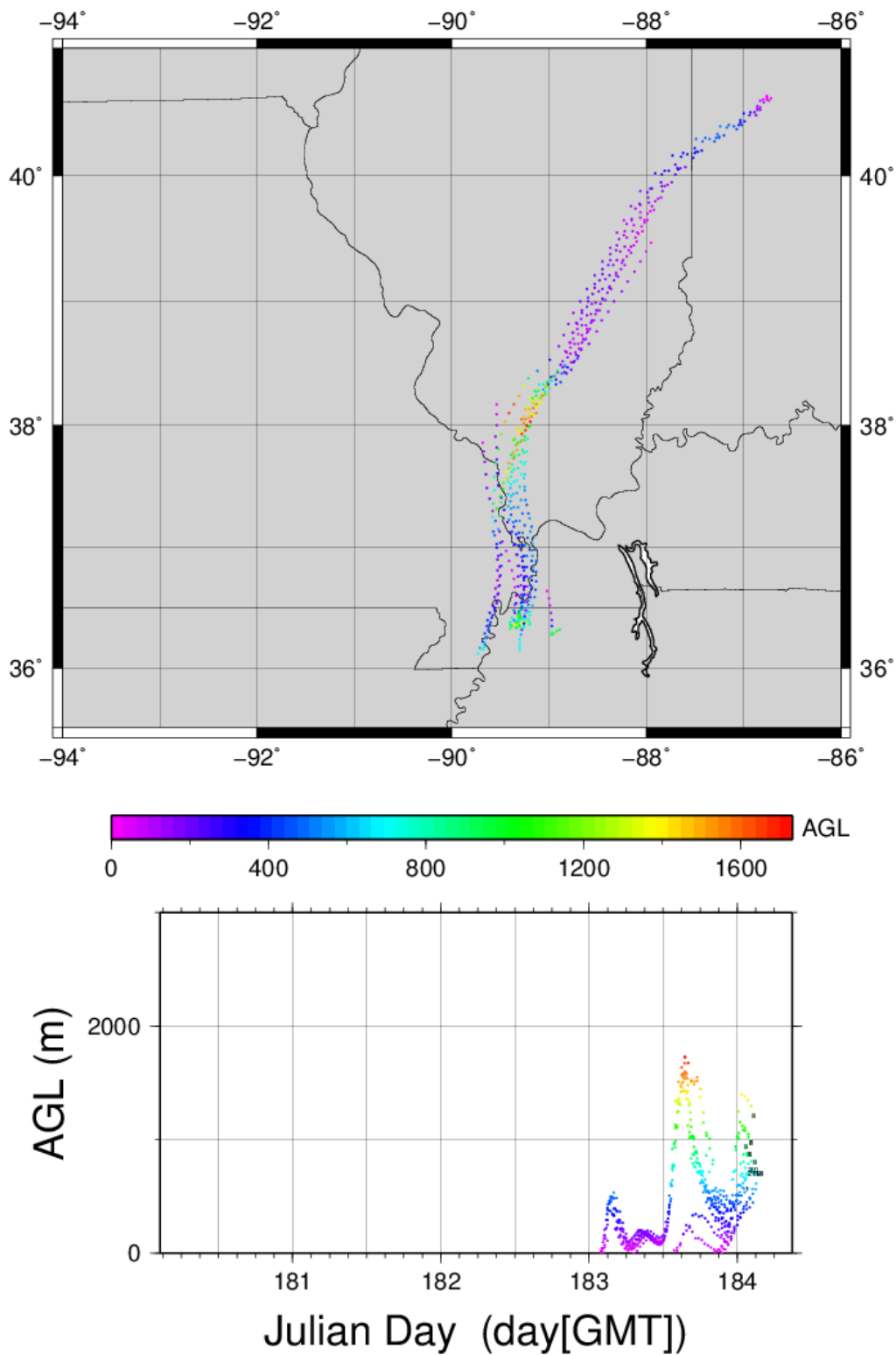
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Figure 10: a backward trajectory analysis for CH₃CN concentration in ppt greater than 400 ppt measured along a SENEX flight on July 03 in: (upper) aerial, and (lower) time vertical cross-sections.

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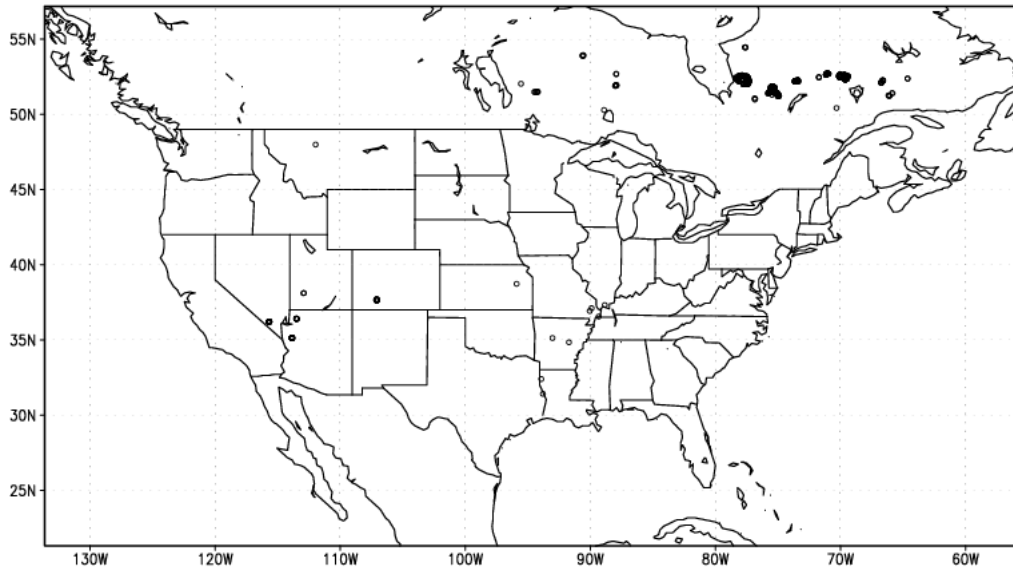
654   **Figure 11a: fire hotspots in hmxhysplit.txt on July 03 2013 as daily composite.**

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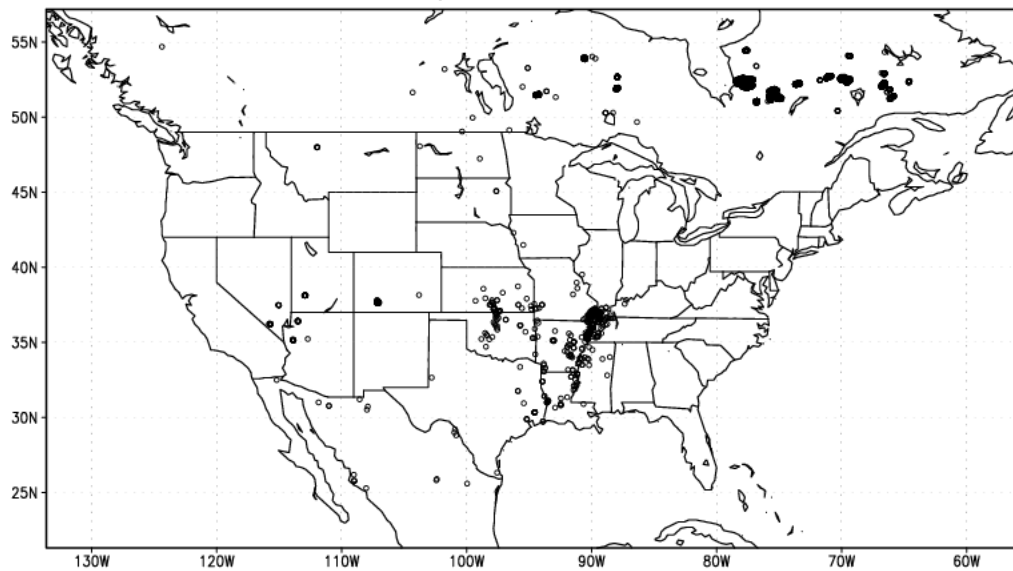
656   **Figure 11b: fire hotspots in hmx.txt on July 03 2013 as daily composite.**

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662 **Tables:**

663 <div align="center">**Table 1: observed and simulated CO (ppb) during NOAA SENEX**</div>

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

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668 <div align="center">**Table 2: identified fire signals from IMPROVE measurements during SENEX**</div>

Site	Date	Concentrations (ug m^{-3})						Ratio (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

669 Notes: (ratios for EC, OC and K > 1.2) **U** (ratio for SOIL < 1.0) **U** (ratios for NO_3^- and SO_4^{2-} < 1.5);

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