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Fusion of Mobile In Situ and Satellite Remote Sensing Observations of Chemical Release Emissions to Improve Disaster Response

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1 **Fusion of Mobile In Situ and Satellite Remote Sensing Observations of Chemical**
2 **Release Emissions to Improve Disaster Response**

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14
15 IL field collected data, analyzed the satellite data and wrote the manuscript. CM analyzed the
16 *in situ* data and made figures. JF helped data collection. XC ran WRF. MF analyzed WRF winds
17 and edited the manuscript and made figures. JM edited the manuscript, DG contributed to the
18 manuscript organization and structure.

19
20 **Abstract**

21 Chemical release disasters have serious consequences, disrupting ecosystems, society, and
22 causing significant loss of life. Mitigating the destructive impacts relies on identification and
23 mapping, monitoring, and trajectory forecasting. Improvements in sensor capabilities are
24 enabling airborne and space-based remote sensing to support response activities. Key
25 applications are improving transport models in complex terrain and improved disaster response.

26 Understanding urban atmospheric transport in the Los Angeles Basin, where topographic
27 influences on transport patterns are significant, was improved by leveraging the Aliso Canyon
28 leak as an atmospheric tracer. Plume characterization data was collected by the AutoMOBILE
29 trace Gas (AMOG) Surveyor, a commuter car modified for science. Mobile surface *in situ* CH₄
30 and winds were measured by AMOG Surveyor under Santa Ana conditions to estimate an
31 emission rate of 365±30% Gg yr⁻¹. Vertical profiles were collected by AMOG Surveyor by
32 leveraging local topography for vertical profiling to identify the planetary boundary layer at ~700
33 m. Topography significantly constrained plume dispersion by up to a factor of two. The observed
34 plume trajectory was used to validate satellite aerosol optical depth-inferred atmospheric
35 transport, which suggested the plume first was driven offshore, but then veered back towards
36 land. Numerical long-range transport model predictions confirm this interpretation. This study
37 demonstrated a novel application of satellite aerosol remote sensing for disaster response.

38
39 **Keywords:** Methane, disaster response, remote sensing, aerosol, plume, atmospheric transport,
40 megacity

42 **1. Introduction**

43 **1.1 Chemical release disasters**

44 Common peacetime anthropogenic chemical release disasters include petroleum spills, e.g.,
45 Deepwater Horizon (Leifer et al., 2012) and chemical process explosions from refineries and
46 other chemical plants (Khan and Abbasi, 1999) can have serious consequences, disrupting
47 ecosystems, society, and causing significant loss of life. Natural chemical release disasters also
48 occur from volcanoes (Schmidt et al., 2015) and other geologic sources (Sigurdsson et al., 1987),
49 with serious implications, too. Moreover, natural disasters often precipitate anthropogenic
50 disasters (Young et al., 2004). For example, the Great East Japan Earthquake caused an oil
51 refinery fire (Dobashi, 2014), while the Northridge 1994 earthquake caused gas releases from
52 134 locations, including two oil refinery releases at 65 km from the epicenter and many natural
53 gas pipeline ruptures and fires (Lindell and Perry, 1997). Mitigation of the destructive impacts
54 relies on identification and mapping, monitoring, and trajectory forecasting. Improvements in
55 sensor capabilities are enabling airborne and space-based remote sensing to support response
56 activities with well-known applications including the Deepwater Horizon oil spill (Leifer et al.,
57 2012) and wildfires (Krstic and Henderson, 2015).

58 In densely populated urban setting, the fate or trajectory of a gas plume from a chemical
59 disaster, such as a refinery release, can pose extreme danger to surrounding downwind
60 communities (Shie and Chan, 2013) and to critical infrastructure, like hospitals, which already
61 could be degraded in the case of earthquake-induced releases. For example, the Northridge
62 Earthquake forced 6 hospitals offline with only 136 critical beds available at one point, while
63 many hospitals suffered internal chemical releases (Lindell and Perry, 1997). Clearly, health
64 risks are significant, yet the main obstacle to effective assessments of population risks often
65 arises from a lack of timely and comprehensive environmental monitoring data (Benjamin,
66 2009).

67 Two current airborne remote sensing systems have been described that can respond to
68 chemical release disasters for a wide range of toxic gases. One is the non-imaging spectrometer,
69 ASPECT (Airborne Spectral Photometric Environmental Collection Technology), which was
70 deployed during the Deepwater Horizon oil spill (Shen and Lewis, 2011). ASPECT provides
71 column data along transects. A second, currently operational system is the thermal infrared (TIR)
72 imaging spectrometer, Mako, which can map gas plumes (Tratt et al., 2014). Its predecessor
73 instrument, SEBASS, was deployed during the Deepwater Horizon oil spill (Leifer et al., 2012).
74 Both TIR imaging systems can detect and quantify a wide range of trace gases.

75 Still, space-based remote sensing has significant advantages. If revisit times are short, they
76 can acquire data globally within an orbit (clear skies permitting), providing initial assessments
77 before airborne or surface mobilization often is feasible and/or during periods when weather may
78 ground airborne assets. Satellites also can observe geopolitically and physically inaccessible
79 locations (Leifer et al., 2012).

80 **1.2. Aliso Canyon Leak Emissions and Fate: Study Motivation**

81 The Aliso Canyon leak was a long-term (~four months) chemical release, primarily
82 comprised of the greenhouse gas, methane (CH₄) (Conley et al., 2016). On decadal timescales,
83 CH₄ affects atmospheric radiative balance far more strongly than carbon dioxide (CO₂), (IPCC,
84 2007, Fig. 2.21), yet large uncertainties remain for many sources (IPCC, 2014). Uncertainty is
85 large for the most important anthropogenic contributor to global budgets, fossil fuel industrial
86 (FFI) emissions (Brandt et al., 2014). Aliso Canyon leak emissions during the first month or so

87 were assessed from multiple airplane flights at 60 tons CH₄ per hour, which is comparable to the
88 entire Los Angeles Basin (Conley et al., 2016). Although regionally significant, these emissions
89 are far less than uncertainties and discrepancy between studies for many budget components at
90 the global level (IPCC, 2014) and even at the California State level (Wecht et al., 2014).

91 In this study we use MODIS (Moderate Resolution Imaging Spectroradiometer) Aerosol
92 Optical Depth (AOD) as an air mass tracer to assess trajectory and thus the fate of released gases
93 from the Aliso Canyon leak. Aerosols are common in many environments (Heintzenberg, 1989),
94 and thus provide a tracer even for chemical releases without aerosol production and release (i.e.,
95 generally no fire). Satellite synoptic imagery, like MODIS, have been used to study urban air
96 quality including mesoscale transport (Engel-Cox et al., 2004); however, ancillary data, such as
97 winds, can be key to interpretation and validation (Engel-Cox et al., 2005).

98 To validate this novel approach, we conducted surveys with a mobile surface platform of
99 fast, highly sensitive *in situ* sensors that can measure a range of trace gases and meteorology
100 (Leifer et al., 2014) to map plume trajectory and fate. Such data, in conjunction with space-based
101 remote sensing, benefit disaster response by improving our ability to model atmospheric
102 transport, while complementing airborne *in situ* data. To our knowledge, this is the first such
103 application for a chemical release, which did not include fire.

104 **1.3 Topography and trajectory**

105 Responders to a chemical disaster need to rapidly identify downwind communities, assess the
106 magnitude of threat and act expeditiously and accordingly. In the case of fires, smoke provides a
107 readily observable atmospheric tracer for comparison with transport models (Krstic and
108 Henderson, 2015). For example, satellite aerosol data are readily available and have been used to
109 track smoke plumes, providing synoptic-scale information (Engel-Cox et al., 2004).

110 However, not all chemical releases include aerosols (smoke), one recent example being the
111 Aliso Canyon natural gas leak in Northern Los Angeles (Conley et al., 2016). The Aliso Canyon
112 release illustrates challenges that exist in plume trajectory mapping and hence forecasting for the
113 complex topography that defines the Los Angeles Basin (Lu and Turco, 1995). Weather in
114 mountainous terrain affects about half the earth's population, as well as half the earth's surface
115 (Meyers and Steenburgh, 2013). Thus, it is unsurprising that effects are particularly complex
116 where mountains overlap dense urban settings.

117 Complex topography affects air quality and atmospheric transport in Los Angeles and other
118 megacities (Gurjar et al., 2008). For practical reasons, application of the precautionary principle
119 for Los Angeles likely is suboptimal – megacity populations are too great to evacuate rapidly,
120 and most, like Los Angeles, have a transportation network that slows to a halt even under normal
121 rush hour traffic. Furthermore, key transportation bottlenecks in Los Angeles coincide with inter-
122 basin airflow pathways with passes referenced by their major highway arteries. Thus, downwind
123 passes, which are likely to transport released, hazardous chemicals, can be rendered unsuitable
124 for evacuation. Although, rapid assessment of most-at-risk communities could improve disaster
125 response decisions, it necessarily requires reasonably accurate and most importantly, timely
126 atmospheric transport predictions on fine to basin scales.

127 In the Los Angeles Basin, the semi-permanent eastern Pacific high-pressure system plays a
128 dominant controlling role in weather. This high-pressure system drives light winds and strong
129 temperature inversions that act as a lid restricting convective mixing to lower altitudes.
130 Additionally, surrounding mountains are physical barriers to inland transport (Lu et al., 1997),
131 albeit imperfect. For example, transport through mountain passes severely impacts air quality in
132 the Mojave Desert (Langford et al., 2010).

133 The Planetary Boundary Layer (PBL) is shallow in the Los Angeles coastal plain and valleys,
134 and grows due to convergence and divergence of winds and downward mixing of air into the
135 PBL (Edinger, 1959). The prevailing flow is from the west (Oxnard Plain) and diverges around
136 the Santa Monica Mountains to flow both along the coast and through the San Fernando Valley.
137 Intersecting the San Fernando Valley are the north-south Santa Susana Mountains that force air
138 in the more northerly portions of the San Fernando Valley to flow along the foot hills (Lamb et
139 al., 1978) including the Aliso Canyon site.

140 An alternate wind pattern of strong offshore flows often occurs in fall and winter, the Santa
141 Ana winds (Hughes and Hall, 2010). Santa Ana winds are strong, mountain lee-side, surface-
142 following winds. Santa Ana winds manifest as mesoscale features associated with mountain
143 gravity waves that drive a strong downward momentum flux in the typical, stably stratified
144 California atmosphere. Santa Ana winds are driven by synoptic-scale pressure and/or
145 temperature gradients between the coast and cold interior desert (Hughes and Hall, 2010). For
146 Santa Ana winds, there also is an acceleration of gap winds leeward (west and south) of the
147 Transverse and Peninsular Ranges (Angevine et al., 2013), reaching up to hurricane strength in
148 some locations (Jones et al., 2010). The Santa Ana winds push the normal sea breeze offshore,
149 which reasserts itself once the Santa Ana winds diminish after typically one to three days (1.5
150 day mean), although Santa Ana winds can persist for as long as five days (Jones et al., 2010).

151 Where plumes are well-behaved (low relief terrain, near steady-state winds, etc.), plume
152 transport and dilution is well-described by the Gaussian plume model (Hanna et al., 1982);
153 however, the Los Angeles Basin topography imposes many non-ideal constraints. In the
154 downwind near field of Aliso Canyon, canyon walls constrain lateral diffusion (Drivas and Shair,
155 1974; Lamb et al., 1978) as well as strongly influencing the lateral wind field. Wind velocities
156 are fairly uniform vertically within the PBL for the downslope Santa Ana wind flow, which
157 follows the terrain (Hughes and Hall, 2010; Cao and Fovell, 2016). There also is a strong
158 constraint on mixing between the top of the PBL and the free troposphere (Hong et al., 2006).

159 In this manuscript, we present the methodology for data collection with additional
160 information in the supplemental material, details on the plume inversion model, and also a brief
161 summary of the numerical trajectory model. Then, *in situ* observations including of the
162 downwind plume transport and vertical profile measurements. We then present satellite aerosol
163 observations that we use to infer far field downwind transport, confirmed by numerical transport
164 model output. Our primary conclusion is that satellite aerosol observations can be leveraged to
165 improve disaster response.

166

167 **2. Methods**

168 **2.1. Study area**

169 The Aliso Canyon storage field is a depleted oil reservoir that serves as the fourth largest in
170 the US (EIA, 2014) and lies at 500-750 m altitude (Fig. 2A) in the foothills of the Santa Susana
171 Mountains (750-1000 m altitude) at the northern edge of the San Fernando Valley (250-290 m
172 altitude) in northern Los Angeles. The land-sea breeze dominates daily winds and typically shifts
173 from nocturnal patterns mid-morning (Lamb et al., 1978). From 23 October 2015 through mid-
174 February, an uncontrolled natural gas leak from the Aliso Canyon storage field (Conley et al.,
175 2016) created an intense CH₄ plume (IPCC, 2014). Overall, fugitive distribution leaks, such as
176 from Aliso Canyon, contribute significantly to the fossil fuel industrial budget (Howarth et al.,
177 2011).

178 **2.2. In Situ Mobile Platform and Survey Approach**

179 Mobile surface atmospheric measurements have been conducted for many years using
180 customized vans (Lamb et al., 1995) or other large vehicle – e.g., camper (Farrell et al., 2013;
181 Leifer et al., 2013); however, the development of cavity enhanced absorption spectroscopic
182 sensors has opened the way for measuring a range of trace gases (Leen et al., 2013) using smaller
183 vehicles without the need for compressed gases – i.e., lower logistical overhead (Leifer et al.,
184 2014; McKain et al., 2015; Yacovitch et al., 2015). Such measurements are complicated in the
185 urban environment by traffic and strong (localized) vehicular impacts. Approaches to mitigating
186 these confounding influences include nocturnal surveys (Farrell et al., 2013), using secondary
187 combustion product gases, such as nitric oxide, total nitrogen oxides, and ozone, to filter data
188 (Leifer et al., 2014), and route selection leveraging the upwind side of traffic arteries under
189 medium to strong cross winds. Absent careful survey design, on-road sources can confound
190 urban data—for example, vehicles are a significant source of CH₄ emissions (Piccot et al., 1996),
191 among other trace gases.



192
193 Fig. 1. Photos of AMOG (AutoMOBILE trace Gas) Surveyor. Upper left inset shows cockpit.

194 The Aliso Canyon leak did not include any high toxicity components. This allowed
195 improvised and safe deployment of AMOG (AutoMOBILE trace Gas) Surveyor to acquire plume
196 measurements. Data also demonstrated the value of such a platform to disaster response by
197 leveraging available-to-mobilize AMOG Surveyor, which has low logistical overhead.

198 Mobile surface CH₄ and meteorology data were collected by AMOG Surveyor (Fig. 1) in the
199 northern Los Angeles Basin on 13 Nov. 2015 to characterize the plume’s downwind evolution
200 (Fig. 2). The AMOG Surveyor was developed to validate satellite greenhouse gas observations
201 (Leifer et al., 2014) and records high quality, fast, meteorology and trace gas concentrations at
202 up to highway speed. Custom software is used by AMOG Surveyor for real-time visualization in
203 the Google Earth environment of multiple data streams to facilitate adaptive surveying. In
204 adaptive surveying real-time data visualization is used to modify the survey to improve science

205 outcomes (Thompson et al., 2015). A range of trace gas analyzers are supported by AMOG
206 Surveyor with the full suite described in the supplementary material; here we only summarize
207 analyzers relevant to this study.

208 Sample air is drawn down a 1/2" Perfluoroalkoxy (PFA) teflon sample line from five meters
209 above ground into a configurable range of gas analyzers by a high flow (30 ft³ min⁻¹) vacuum
210 pump (Edwards, GVSP30). The sample line connects to several instruments including a Fast-
211 flow, enhanced performance Greenhouse Gas Analyzer (FGGA), which uses Integrated Cavity
212 Off Axis Spectrometer-Cavity Ring Down Spectrometer (ICOAS-CRDS) and measures CO₂,
213 CH₄, and water vapor (H₂O) at up to 10 Hz (Model 911-0010, Los Gatos Research, Inc.).

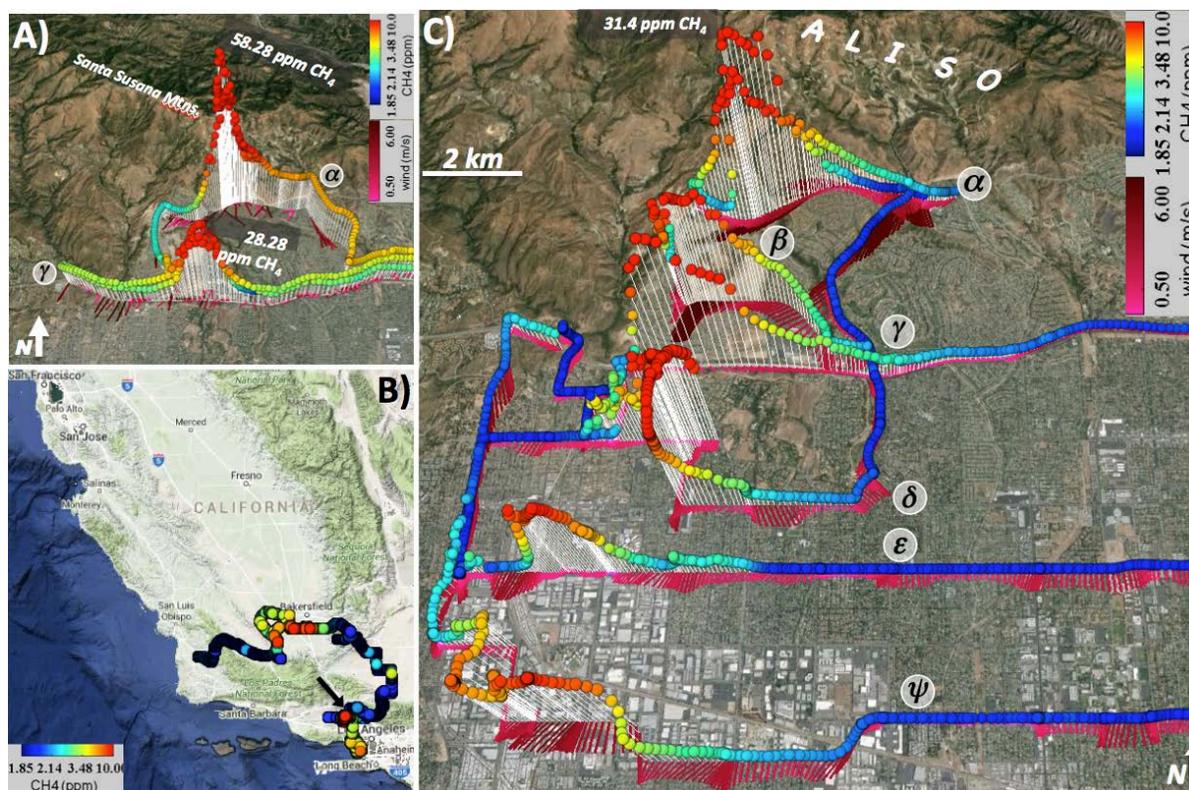
214 A sonic anemometer (VMT700, Vaisala) mounted 1.4-m above the roof measures two-
215 dimensional winds. Recent science AMOG Surveyor system improvements beyond Leifer et al.
216 (2014) include a fast thermocouple (50416-T, Cooper-Atkins) and a high accuracy (0.2 hPa)
217 pressure sensor (61320V RM Young Co.). Thermocouples (Type T) are digitized at ±0.03°C
218 (CB-7018, Measurement Computing), which also digitizes the solar insolation sensor at 16 bit
219 and one hertz (CB-7017, Measurement Computing). Position information is critical to accurate
220 real winds and is provided at 10 Hz by redundant (two) Global Navigation Satellite Systems
221 (19X HVS, Garmin) that use the GLONASS, GPS, Galileo, and QZSS satellites for improved
222 performance.

223 The use of real-time traffic and familiarity with the study area aids navigation, while real-
224 time wind visualization can be used to ensure driving on upwind side of streets and highways.
225 The impact of dense urban structures on winds can be reduced by filtering for specific open areas
226 such as parking lots, fields, etc. in post-processing. Additionally, intersections with idling cars
227 create local, near-surface exhaust clouds. This was addressed by timing approaches to
228 intersections to allow idling cars and their emission clouds to flush downwind, and by collecting
229 air samples at slow driving speed from five-m height. Although nocturnal data collection avoids
230 many urban challenges (Leifer et al., 2013), the nocturnal urban atmosphere typically features
231 low wind speeds and a very shallow PBL, making modeling highly challenging (Finn et al.,
232 2008). An additional urban challenge arises from dense multi-story structures, where the road
233 grid channels surface winds. However, once a plume diffuses above the structures it can drift
234 freely but will re-enter the road grid through downward diffusion.

235 *In situ* surveys included the collection of vertical profile data to identify the PBL by
236 leveraging nearby topography. Specifically, AMOG Surveyor drove into the nearby San Gabriel
237 Mountains, approximately 10-20 km to the east. Profile surveys used small, sparsely trafficked
238 roads. Still, there was some traffic, which was addressed by AMOG Surveyor pulling alongside
239 the road for one to two minutes when catching up to a slower vehicle.

240 **2.3. Plume inversion and uncertainty**

241 There are two approaches to assess emissions, either by an assimilation inversion model
242 based on a range of stationary station measurements (Jeong et al., 2012; Jeong et al., 2013b), or a
243 direct assessment approach (White et al., 1976; Karion et al., 2013; Peischl et al., 2015). Direct
244 assessment has advantages over inversion approaches. Specifically, direct approaches allow
245 explicit evaluation of uncertainty with no need for an a-priori emission spatial distribution, nor
246 for the ability to model accurately atmospheric transport. The latter two aspects challenge
247 assimilation approaches, particularly for areas of complex topography, regions with poorly
248 characterized (or unknown) sources. Furthermore, challenges arise where temporal variability in
249 winds and emissions require data to be collected sufficiently rapidly with adequate data density
250 to address fine-scale structure.



251
 252 Fig. 2. A) Pre-survey methane (CH₄) concentrations and winds downwind of the Aliso Canyon
 253 leak, collected 05:06-05:39 PST, 13 Nov. 2015. Peak plume transect concentrations labeled. B)
 254 California map showing all collected data 13-14 Nov. 2015. Black arrow shows Aliso Canyon
 255 location. C) Methane, CH₄, and wind observations for the Aliso Canyon leak in the San
 256 Fernando Valley, CA, collected 10:40-15:10 PST, 13 Nov. 2015. Note, CH₄ color bar is
 257 attenuated to capture spatial concentration structure near ambient. Data keys on panel.

258 Total emissions (E) were estimated by two different direct approaches, a Gaussian plume
 259 inversion (E_{Gauss}), and a well-mixed PBL integration (E_{Mixed}).

260 Plume inversion was performed on purely east west transects (no north-south jogs).

261 Inspection of the “clean” transects (γ and ϵ), i.e., transects that were purely east west without
 262 north-south jogs (dictated by road accessibility) used the curvfit tool in MatLab (Mathworks,
 263 MA) to fit dual Gaussian functions (Fig. 2C) to the anomaly concentration (C') for each transect.
 264 C' was calculated from the average of the lowest values to the west of the plume (east of the
 265 plume, CH₄ concentrations were influenced by urban sources).

266 The Gaussian functions were used to segregate data between the different plumes, and were
 267 not used in the Gaussian plume model. The dual plume character was consistent with
 268 observations at the most northerly roads that concentrations peaked in front of two canyons to
 269 the south of the source (Fig. 2). This spatial structure was apparent in all transects. A sharp,
 270 narrow plume was fit to transect ϵ , which was assessed as having a local (non-Aliso) source, and
 271 was segregated out of C' as used in the model.

272 Transect wind speeds were acceleration-filtered ($>1 \text{ m s}^{-2}$) and then rolling-median time-
 273 filtered (10-s time window). Finally, the upper 10% of wind speeds were used to estimate the
 274 wind speed based on the wind probability distribution for each transect. This accounts for the
 275 weaker winds reflecting the influence of buildings, trees, etc., and was validated during a vertical

276 profile inter-comparison between AMOG Surveyor and an airplane data set collected in the
277 Sierra Nevada Mountains. This approach also accounts for extending wind speeds from three to
278 10 m above ground heights (Leifer, unpublished data).

279 The Gaussian plume model is based on Hanna et al. (1982) and error minimized between the
280 modeled and measured C' , for the along-wind, transverse, and vertical dimensions, x , y , z ,
281 respectively, to estimate E and is:

$$282 \quad C'(x, y, z) = E \frac{\exp\left(-y^2/2\sigma_y^2\right)}{(2\pi u \sigma_z \sigma_y)} \left(\exp\left(-z^2/2\sigma_z^2\right) + \exp\left(-(z+h)^2/2\sigma_z^2\right) \right),$$

283 where h is plume origin height, u is wind speed, and σ_y and σ_z are given by:

$$284 \quad \sigma_y = k0.11\sqrt{1 + x/10^4}; \quad \sigma_z = k0.08\sqrt{1 + x/2 \times 10^4},$$

285 from (Hanna et al., 1982) for Briggs Turbulence and stability class three, and k is an added factor
286 between zero and one that accounts for constraint of the plume's lateral dispersion due to
287 topography after Bierly and Hewson (1962). Stability class three is unstable with strong solar
288 insolation and moderate to strong winds. The emission height (h) was set at 150 m to address the
289 plume's initial buoyant rise and injection at altitude. However, the flux is very weakly sensitive
290 to h at the distances of the plume transects. Although the source location was known, the origin
291 for the Gaussian plume at downwind distance (D) was allowed to vary because the canyons have
292 a "channelizing" effect on the plume, preventing lateral dispersion (Angell et al., 1972; Lamb et
293 al., 1978). This is equivalent to a "virtual origin" for the plume close to the canyon mouth (where
294 it exits onto the alluvial tilted plain of the north San Fernando Valley). The wind speed was
295 approximately four meters per second for sunny conditions, thus, the inversion calculation used
296 stability class three (Hanna et al., 1982). Table 1 provides Gaussian model parameters.

297 The value of E for plume first was calculated by averaging E_{Gauss} for both transects with
298 E_{Mixed} for transect ϵ and was 365 Gg CH₄ yr⁻¹. However, a best estimate for E was calculated
299 using a scenario approach (Shakhova et al., 2014), which also was used to derive the uncertainty
300 (Supp. Section S.2). The scenario approach is a simplified Monte Carlo where the probability
301 distribution function that normally would be sampled for the Monte Carlo simulations is
302 assumed uniform, but quantized. For each scenario, low, observed, and high wind speeds of
303 three, four, and five m s⁻¹, respectively, were chosen for the plume inversion, and represent the
304 envelope of observations. This uncertainty scenario is based on the reality that wind speeds only
305 are known (measured) at one point and time and not along the entire path of travel, over which
306 they certainly vary; albeit, within limits. The scenarios also considered that the "source" distance
307 is uncertain, as it is a "virtual distance," due to the effect of topographic control on reducing the
308 lateral turbulence (factor k). D was set at low, high, and best values of $\pm 18.5\%$ (± 1 km at transect
309 ϵ) for each of the two transects based on estimated reasonable limits for the location. For each of
310 the nine scenarios run for each plume on each transect, the inversion algorithm (as above)
311 minimized the error to derive the values for k and E_{Gauss} .

312 2.4. MODIS aerosol optical depth

313 Satellite AOD from the Terra and Aqua MODIS satellites was downloaded and gridded from
314 the satellite granule pixel locations to a uniform latitude-longitude coordinate system using the
315 MatLab (v2015b, Mathworks, MA) sparse interpolation routine, (scattered interpolant) with the
316 "natural" setting. This interpolation routine addresses the retrieval sparseness or non-uniformity
317 of the AOD data, while also ensuring the interpolation goes through each data point. Data were

318 sparse for a number of reasons, include clouds, quality flags, and no retrieval. Only data of the
319 highest quality flag were used with successful retrieval density varying across the scene.

320 **2.5. Weather Regional Forecast model**

321 To interpret the spatial distributions of AOD enhancements, the Weather Regional Forecast
322 (WRF) model, version 3.6.1, was run in a series of four nested domains ranging from 36-km over
323 Western US down to 1.3-km resolution, providing wind fields and PBL thicknesses over a
324 domain covering the South Coast Air Basin that includes Aliso Canyon. The WRF model was
325 run with time averaging adapted for atmospheric trace gas transport (Skamarock et al., 2008;
326 Nehr Korn et al., 2010; Jeong et al., 2013a) over California. Here, we employed boundary and
327 initial conditions from the North American Regional Reanalysis (NARR) dataset (Mesinger et
328 al., 2006). We parameterized WRF to use 50 vertical levels, applied the MYNN2 boundary layer
329 physics (Nakanishi and Niino, 2006) and unified NOAA model for land surface properties (Chen
330 and Dudhia, 2001). This minimizes errors in boundary layer meteorology. We computed each
331 day of simulation in a separate 30-h run with an initial six-hour spin-up.
332

333 **3. Results**

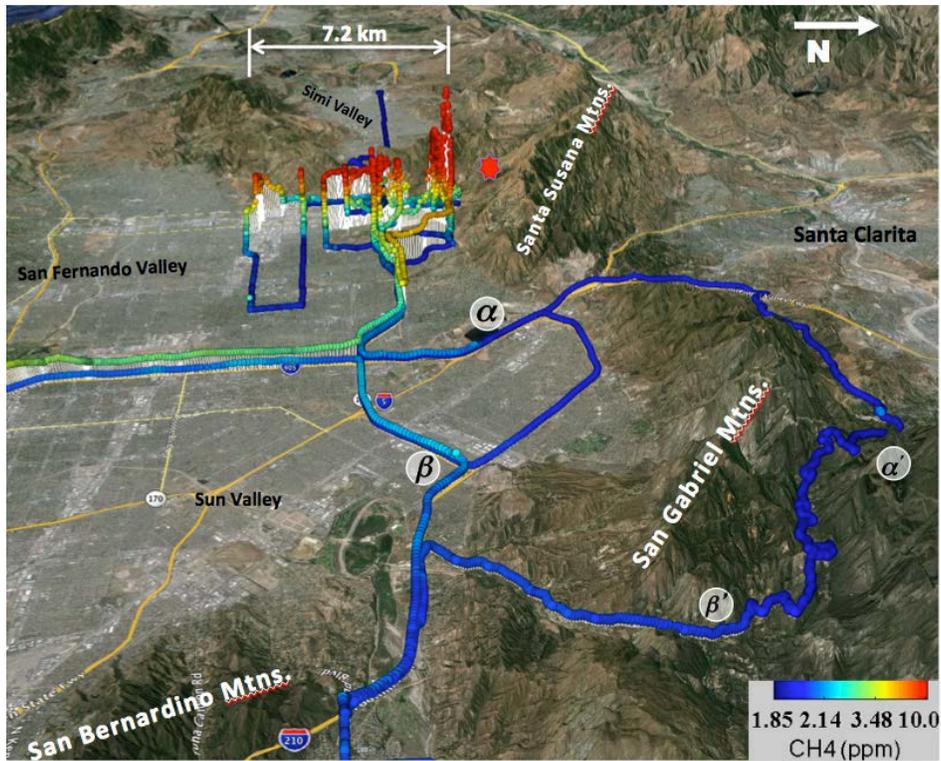
334 **3.1. Pre-survey observations**

335 Prior to the main survey, a pre-survey (Fig. 2A) was performed at ~05:00 LT (Local Time)
336 when traffic on Los Angeles highways is light. The pre-survey was conducted to understand area
337 survey constraints from traffic and terrain for predicted winds, which already exhibited Santa
338 Ana wind strengths ($u = 5$ to >10 m s⁻¹) at altitudes above 400 m. For example, heavy traffic
339 prevents surveys on US-101 (both directions) after ~06:00 LT.

340 Pre-survey CH₄ concentrations to 58 part per million (ppm) were observed at 05:17 LT
341 downwind of the principal canyons that guide plumes in the near field (transect α in Fig. 2A). An
342 extended weaker plume (CH₄ > 6 ppm) was observed to the east of the main plume,
343 representative of nocturnal transport down a different canyon. At this hour (stably stratified,
344 nocturnal wind patterns), strong Santa Ana winds were observed primarily in front of canyon
345 outflows and showed significant spatial heterogeneity. Despite strong winds (to 9.7 m s⁻¹) and a
346 source distance of several kilometers, these values were significantly higher than almost all
347 surface observations obtained in tens of thousands of AMOG Surveyor data across Southern
348 California.

349 **3.2. Main survey**

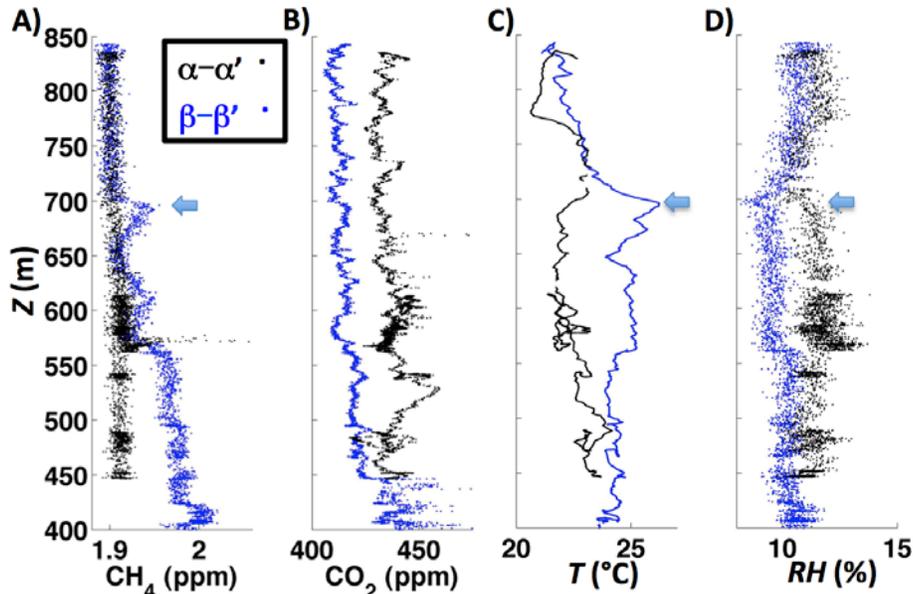
350 Mobile surface survey data of the Aliso CH₄ plume were collected mid-morning, 13 Nov.
351 2015 to characterize the plume's downwind evolution (Fig. 2C). By mid-morning, online
352 weather information (www.weatherunderground.com) indicated that the nocturnal weather
353 patterns had shifted to daytime conditions. The survey repeatedly transected the plume at
354 multiple downwind distances from the source (y) from two to nine kilometers (Fig. 3).



355
 356 Fig. 3. Methane (CH₄) data collected in the San Fernando Valley and up into the San Gabriel
 357 Mountains to collect atmospheric vertical profile information. Red star shows leak location. Data
 358 key, vertical profile locations (α - α' is ascent profile, β' - β is descent profile), and size scale on
 359 figure.

360 **3.3. Atmospheric profile characterization**

361 Aside from collecting downwind data for the Aliso Canyon leak, three vertical profiles were
 362 collected into the San Bernardino Mountains (Fig. 3) to elevations of 830 m and 1.4 km above
 363 mean sea level (AMSL, all altitudes are AMSL). Two profiles were conducted before the survey,
 364 and one afterwards while transiting to near the Edwards Air Force Base in the Mojave Desert.
 365 The profiles (Fig. 4) showed air in the lower Los Angeles Basin had enhanced CH₄ and CO₂,
 366 largely constrained to a layer extending to ~570 m, although it is important to note the influence
 367 of winds down the I-5 Pass (α - α'). However, the temperature profiles both showed that AMOG
 368 Surveyor entered distinct upper level air at about 700 m, where the relative humidity also showed
 369 a minimum. Also, there was a slight (~50 ppb) enhanced CH₄ in a thin layer at this altitude,
 370 which also was the top of an inversion layer, observed on the descending transect. Note, the
 371 more enhanced CO₂ anomalies from 400-450 m altitude are influenced by traffic on the I-5;
 372 however, the small road driven up into the San Bernardino Mountains had almost no traffic.



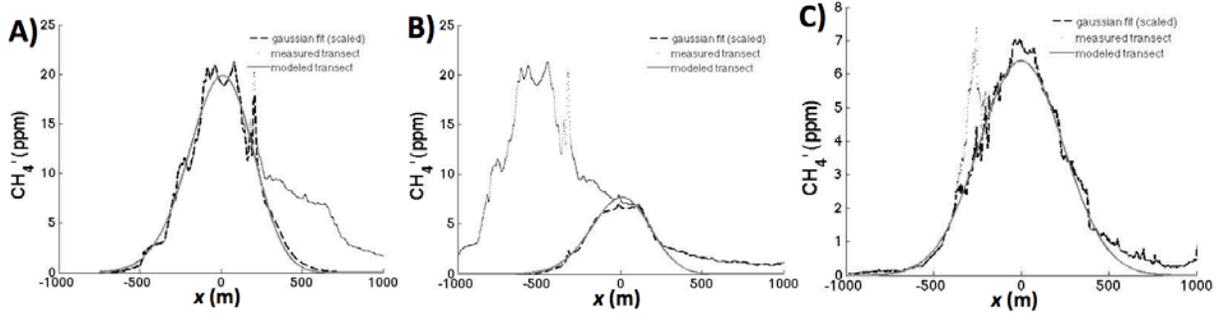
373
 374 Fig. 4. AMOG altitude (z) profile data into the San Bernardino Mountains for A) methane (CH₄),
 375 B) carbon dioxide (CO₂), C) temperature (T), and D) relative humidity (RH). Blue arrows
 376 highlight features showing top of the planetary boundary layer. Vertical profiles ($\alpha - \alpha'$ is ascent
 377 profile, $\beta' - \beta$ is descent profile) are labeled as identified on Fig. 3. Data key on panel A.

378 Vertical profiles were collected in the San Bernardino Mountains before and after the main
 379 survey and showed a stable PBL (690-720 m), which grew only a few dozen meters over several
 380 hours (Figs. 3 and 4). Although the PBL was identified *below* the leak altitude, Santa Ana winds
 381 follow topography (Hughes and Hall, 2010), driving the plume downslope, while also
 382 minimizing the potential for significant buoyant rise.

383 3.4. Plume inversion

384 Plume inversion (Hanna et al., 1982) based on error minimization was conducted on the two
 385 downwind “clean” transects (γ, ϵ) – east-west that were along a straight pathway – in some cases,
 386 available roads prevented straight transects. The inversion used a model that incorporated
 387 topographic control on plume dispersion due to being in a canyon (Drivas and Shair, 1974; Lamb
 388 et al., 1978). These transects were well described by dual Gaussian functions (Table 1, Fig. 5).
 389 The dual plume character was consistent with observations at the most northerly roads that
 390 concentrations peaked in front of two canyons to the south of the source (Fig. 2), a spatial plume
 391 structure that was apparent in all transects.

392 The closer transect (γ) had good agreement between E_{Mixed} and E_{Gauss} , within the uncertainty
 393 of E_{Gauss} , where E_{Gauss} is the Gaussian plume inversion and E_{Mixed} assumes a well mixed PBL.
 394 E_{Mixed} used the observed 700 m PBL (Fig. 3) and assumed constant winds with altitude. Observed
 395 wind profiles for Santa Ana winds show fairly uniform distribution with height on the downslope
 396 flow portions of the plume, although Santa Ana winds weaken dramatically once out onto the
 397 plains, where the wind profile becomes significantly non-uniform (Hughes and Hall, 2010). This
 398 likely explains the worse agreement between E_{Mixed} and E_{Gauss} .



399
 400 Fig. 5. A) Methane (CH_4) anomaly concentration (CH_4') profiles, with respect to transverse
 401 distance (x) Gaussian functional fit to data, and Gaussian plume model fit for A) transect γ for
 402 main plume, and B) transect γ fit for secondary plume, and C) fit for the plume on transect ϵ .
 403 Data key on figure.

404

405 Table 1. Best scenario estimated flux and parameters

406 Transect	D	h	u	S	k	PBL*	E_{Gauss}	R^2	E_{Mixed}
407 (-)	(km)	(m)	(m s^{-1})			(m)	(Gg yr^{-1})		(Gg yr^{-1})
408 γ	2.7	150	4.0	3	0.75	700	$457 \pm 25\%$	0.99, 0.90	405
409 ϵ	5.5	150	4.0	3	0.50	700	$282 \pm 30\%$	0.97	162

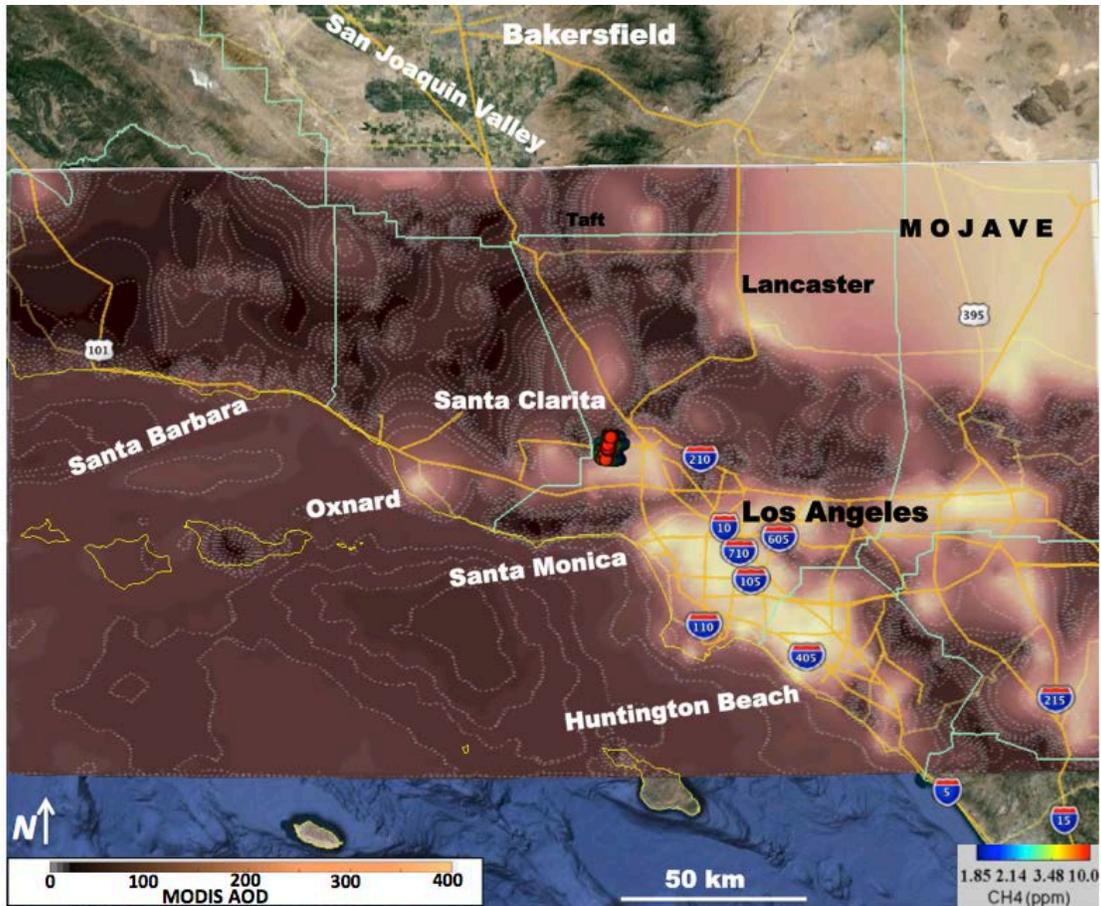
410

411 Key: D – distance to source, h – emission height, u – wind speed, S – Briggs Stability Class, PBL
 412 – Planetary Boundary Layer – altitude in meters above mean sea level, R^2 is the model fit
 413 correlation coefficient, E_{Gauss} – Gaussian plume emission estimate, E_{Mixed} – well mixed PBL
 414 emission estimate.

415 *above ground level.

416

417 Additional issues arise from the lateral wind profile. Within and near the canyon, including
 418 the Porter Ranch community, winds and CH_4 exhibit similar large-scale spatial structure under
 419 strong topographic influence; as evidenced by “ k ” being much less than one ($k = 1$ implies a non-
 420 topographically constrained plume). However, for the more distant transect, the plume sprawls
 421 over areas with distinct wind regimes. Plume inversion confirmed the extreme strength of the
 422 Aliso Canyon leak emissions (Table 1).

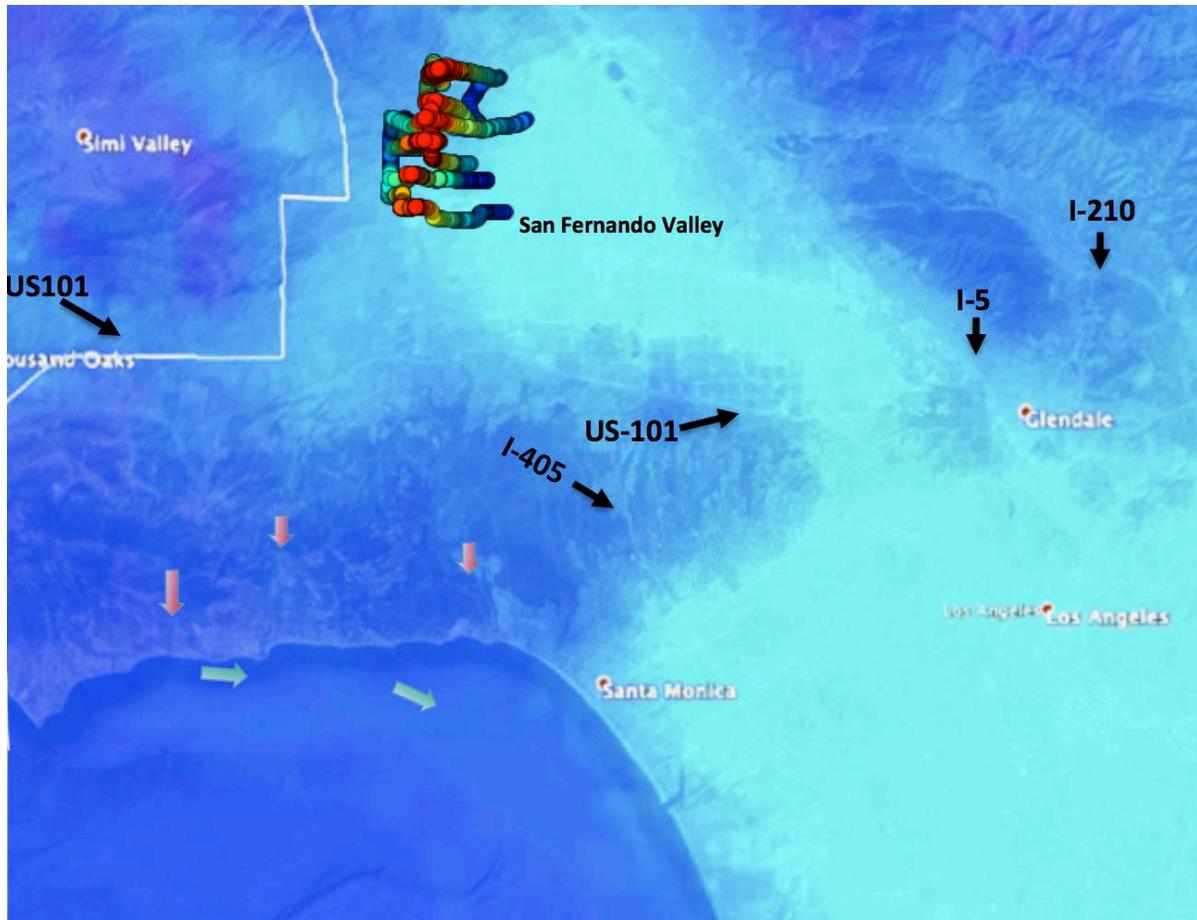


423
 424 Fig. 6. Aerosol Optical Depth (AOD) from MODIS for 2055 UTM, 13 Nov. 2015, for southern
 425 California. Also shown is the Aliso Canyon plume methane (CH₄). Data keys on figure.

426 **3.5. MODIS Aerosol Optical Depth**

427 For this analysis, MODIS, Terra and Aqua, satellite data were obtained for 13 Nov. 2015 for
 428 Southern California, although a longer time set of these data were obtained and reviewed. The
 429 specific aerosol product used was the Level 2, “Image Optical Depth Land and Ocean,” product
 430 (MOD04_3K), for the MODIS data collection 6 and were downloaded from NASA LAADS
 431 (Level 1 and Atmosphere Archive and Distribution System). Specifically, MODIS 250-m
 432 reflectance and the three kilometer aerosol optical depth (AOD) for 0.55 nm products (Levy et
 433 al., 2010) as well as the cloud mask and aerosol type were downloaded and then post-processed
 434 in MatLab (Mathworks, MA). Maps of AOD were visualized with a linear color scale to
 435 emphasize variations for low columns, and any quality-flagged pixels were set transparent. Maps
 436 of AOD then were brought into Google Earth to overlay with *in situ* data.

437 The AOD map (Fig. 6) shows notable enhancements in the Los Angeles Basin and San
 438 Fernando Valley with low AOD for mountainous regions to the north and northwest of Los
 439 Angeles. A map with the AOD contrast enhanced shows spatial structural details that highlight
 440 the presence of enhanced AOD in the coastal mountain passes (red arrows, Fig. 7). Note these
 441 mountain passes are not transportation routes. The fine structure in the AOD map suggests that
 442 transport veers sharply to the east offshore, based on an east-west spatial structure (below green
 443 arrows, Fig. 7). Figure 7 has high contrast enhancement to illustrate AOD spatial structure in the
 444 mountain passes and over the ocean.

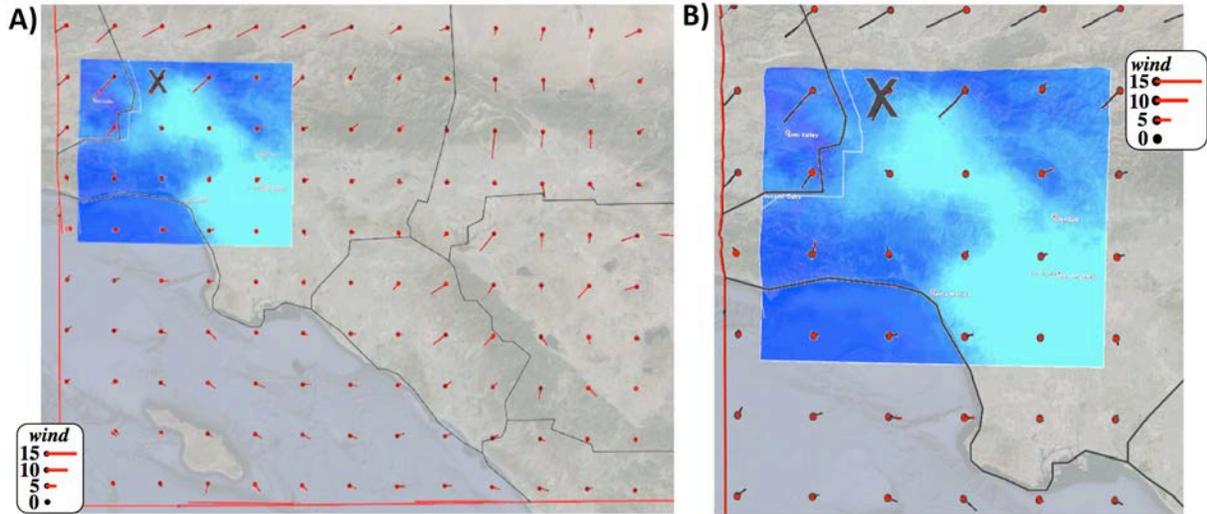


445
 446 Fig. 7. Contrast enhanced to show overall MODIS aerosol optical depth (AOD) structure for 13
 447 Nov. 2015 for northwest Los Angeles and the San Fernando Valley. AOD contrast highly
 448 saturated to bring out spatial structure in passes and over oceans. Pale green arrows lie
 449 immediately north of the offshore AOD structure, which exhibits an east-west orientation and is
 450 shown to illustrate airflows. Major traffic arteries through mountain passes are labeled with
 451 relevant highway and black arrows. Red arrows shows three different plume outflows, the
 452 easternmost corresponding to downwind of the Aliso Canyon leak plume. Methane (CH₄) data
 453 shown for spatial reference. See Fig. 3 for CH₄ data and CH₄ data key. See Fig. 6 for AOD data
 454 with AOD data key.

455 **3.6. Modeled winds and plume transport**

456 Observed plume trajectory overlapped well with MODIS AOD (Fig. 6), which clearly showed
 457 enhanced AOD in passes from the San Fernando Valley to the Pacific Ocean. The contours of
 458 AOD (Fig. 6) strongly suggest canyon outflow to the Pacific Ocean and offshore, followed by
 459 easterly onshore transport across the Santa Monica Bay and towards coastal Los Angeles
 460 communities. The possibility that the offshore spatial structure related to transport was
 461 investigated further through WRF numerical simulations (Fig. 8), which showed that southward
 462 winds through the passes (continuing in the same direction as observations) veered to the east
 463 over the Pacific Ocean. Specifically, WRF simulations captured the shift from offshore Santa
 464 Ana winds to prevailing westerly winds. Additionally, WRF showed that this wind pattern

465 persisted into later in the day (14 Nov. 2015, 0100 UTM) allowing time to transport Aliso
466 Canyon leak CH₄ back onshore.



467
468 Fig. 8. Weather Regional Forecast (WRF) modeled surface (100 m AGL) winds, for 13 Nov.
469 2015, 2100 UTM. A) Large area view showing winds for much of the Los Angeles Basin. Also
470 shown is the Aerosol Optical Depth (AOD) map from Fig. 7 for reference only. B) Zoomed in
471 study area.

472

473 4. Discussion

474 4.1. Improving transport understanding

475 Events such as the Aliso Canyon leak are tracer experiments such as once were common with
476 SF₆ (Lamb et al., 1978). Today, new *in situ* sensors and remote sensing technology can leverage
477 such events to understand better atmospheric transport. In the case of the Aliso Canyon leak, the
478 release occurred in the complex wind flow patterns of a megacity sprawling over terrain with
479 notable topographic relief.

480 Plume dilution was slow for Santa Ana wind conditions (Fig. 2C), which are frequent in Los
481 Angeles during the fall and winter seasons (Abatzoglou et al., 2013). Specifically, $C_{CH_4}(y \sim 2$
482 km) decreased by just half at $y \sim 10$ km. The explanation partly lies in the constraining impact of
483 canyon walls, which reduces significantly the lateral diffusion rate ($k < 1$), and topographic
484 forcing (Angell et al., 1972; Lamb et al., 1978). In future chemical release accidents of a highly
485 toxic gas, dilution with distance cannot be a priori assumed to lower risk rapidly, with even
486 distant communities potentially remaining at risk.

487 The Aliso Canyon leak surface survey required many hours to characterize the local plume
488 (to $y \sim 10$ km) and PBL. Airplane *in situ* is far faster (at least for a highly maneuverable
489 airplane), characterizing plumes above the surface and even over the ocean, but invariably
490 intersects the many controlled airspaces in a megacity like Los Angeles. Moreover, it is the
491 surface concentration that has serious consequences for human health. Thus, surface data can add
492 to airborne data at far lower logistical costs.

493 4.2. Satellite Observations

494 Ideally, remote sensing can help. The ideal response instrument would be a geostationary
495 instrument with high spatial resolution and selectivity for the released gas, providing near real

496 time observations of fate trajectory and emission strength. Geostationary instruments can dwell
497 on an area, unlike low earth orbit satellites (Zhang and Kerle, 2008).

498 To characterize a strong CH₄ leak, such as from Aliso, a CH₄ mapping satellite with coverage
499 and resolution comparable to the OCO₂ satellite (Crisp et al., 2010), which observes only CO₂
500 (at 70-m resolution), is needed. Unfortunately, no CH₄ satellite instrument with kilometer or
501 better resolution currently orbits, nor is one planned for near-future launch. Moreover, there
502 currently is no such spacebased instrument for any of the numerous toxins (e.g., benzene,
503 toluene, etc.) that could be released. Airborne remote sensing has an important advantage in that
504 it avoids entering toxic plumes where *in situ* measurements could pose unacceptable risks to
505 responders.

506 Numerical models can aid response decisions and thereby help fill the lack of a satellite trace
507 gas instrument for plume mapping. However, wind flow complexity related to topography
508 provides major challenges to interpretation of both *in situ* data and numerical models. Thus,
509 validation is critically important. Atmospheric aerosols, which are readily remote sensed from
510 space, provide a good tracer to validate model predictions. Satellite trajectory tracing of aerosols
511 (Engel-Cox et al., 2005) applies directly to refinery or other chemical plant fires where aerosol
512 generation accompanies hazardous gas emissions (Khan and Abbasi, 1999). Nevertheless,
513 because urban aerosols are common (Hayes et al., 2013), they provide a readily available air
514 mass tracer even for incidents that do not include fire, and thus do not generate aerosols.
515 Additional aerosol map cross-validation can be provided from the space-based lidar, CALIOP
516 (Cloud-Aerosol Lidar with Orthogonal Polarization). The CALIOP sensor has been used to study
517 volcanic plumes (Vernier et al., 2013). Additional validation can come from airborne *in situ* and
518 remote sensing of aerosols.

519 The Santa Ana winds drive a southward airflow across and out of the San Fernando Valley
520 through mountain passes, highlighted in the MODIS AOD (Fig. 7). This validated the WRF
521 simulations and illustrates how important topography is to atmospheric transport in the Los
522 Angeles Basin (Drivas and Shair, 1974). Notably, strong AOD enhancements occurred in the
523 main transport corridors that traverse passes within the Los Angeles Basin, such as US-101, I-5,
524 and I-215 (Fig. 7). Given that normal rush hour traffic grinds to a standstill, the suitability of
525 evacuation routes that use these passes, which also may conduct chemical plumes, merits
526 consideration. Ancillary data, such as winds, are key, as elevated AOD does not mean transport.
527 For example, traffic within the passes and *in situ* chemical production certainly produce local
528 aerosols.

529 A southward offshore flow, which is typical for Santa Ana winds (Trasviña et al., 2003), was
530 illustrated by the MODIS AOD. This flow then veered towards the prevailing eastwards wind
531 direction ~10 km offshore. This drove the plume towards densely populated coastal communities
532 near Los Angeles airport. If the disaster had been a refinery emission of highly toxic gas,
533 validation of numerical model predictions would be key for responders assessing which
534 communities needed the most immediate evacuation.

535 Incorporating satellite aerosol remote sensing data into disaster response plans and decision-
536 making requires short latency and rapid revisit times: MODIS Level 1 data latency is 70 minutes,
537 but Level 2 aerosol products have one day latency. Therefore, near real-time products need
538 development. Geostationary aerosol products from GOES (Geostationary Operational
539 Environmental Satellite)(Weber et al., 2010) or the planned TEMPO (Tropospheric Emissions:
540 Monitoring of Pollution) mission can provide half hour or hourly daylight data for North
541 America, respectively (Chance et al., 2013). The TEMPO mission also will provide other

542 potentially contributory satellite data related to air quality trace gases, such as ozone. This study
543 showed a need for improvements in urban real-time AOD retrieval algorithms, where AOD
544 density (despite high quality flags) was non-ideal.
545

546 **5. Conclusion**

547 Characterization of the plume from Aliso Canyon was performed by surveys with the
548 AutoMOBILE trace Gas (AMOG) Surveyor, which measured mobile surface *in situ* CH₄ and
549 winds under Santa Ana conditions. Analysis yielded an estimated annualized emission rate of
550 365±30% Gg CH₄ yr⁻¹. Plume dispersion was constrained significantly by topography, reduced
551 by up to a factor of two. Local topography was leveraged by AMOG Surveyor to provide vertical
552 profiles that were used to identify the planetary boundary layer at ~700 m. Observations showed
553 the plume was transported towards passes in the coastal Santa Monica Mountains. To understand
554 the far field fate, satellite aerosol optical depth was mapped and suggested the plume flowed
555 offshore before veering eastwards back towards shore. This interpretation was validated by
556 comparison with a numerical model.

557 This study demonstrated and validated the novel application of satellite aerosol remote
558 sensing for disaster response. Currently and for the near future, there is no satellite instrument
559 that can map any of the numerous toxins (e.g., benzene, toluene, etc.) that a chemical release
560 disaster can emit. Thus, satellite aerosol remote sensing can provide a readily available proxy
561 tool to provide synoptic scale information on the fate of co-transported toxins from a release.

562 The use of a car based survey platform was novel and has logistical advantages in terms of
563 ease of mobilization. However, car systems are constrained to roads, unlike airplanes, which can
564 easily fly vertical profiles. Ideally, combined surface and airborne data are collected to provide a
565 complete characterization of the atmosphere from the surface where injury occurs to the top of
566 the PBL. Given that airborne data were not collected in tandem with this AMOG Surveyor
567 deployment, local topography was leveraged to provide vertical profiles.

568 Aerosol remote sensing is of high priority to climate, safety, health, and atmospheric
569 corrections for satellite instruments. Thus, including a priori science requirements for disaster
570 response science requirements into the design considerations for future aerosol remote sensing
571 instruments and platforms (airborne and space-based) can improve understanding of urban
572 atmospheric transport. Leveraging these remote sensing tools requires ensuring disaster response
573 scientific requirements contribute to instrumentation and platform design in terms of sensitivity,
574 resolution, and revisit times, (satellite and airborne). Equally important, aerosol products need
575 incorporation into response planning. This would allow future instruments to contribute to
576 mitigating the serious consequence of chemical release disasters.
577

578
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588			
589			
590	Table of Nomenclature		
591	AOD	(-)	Aerosol optical depth
592	C	(ppm)	Atmospheric concentration
593	C'	(ppm)	Atmospheric concentration anomaly
594	CH_4'	(ppm)	Atmospheric CH_4 concentration anomaly
595	D	(m)	distance downwind from the source
596	E	(mol/s)	Emissions
597	E_{Gauss}	(mol/s)	Emissions derived by the Gaussian approach
598	E_{Mixed}	(mol/s)	Emissions derived by the mixed PBL approach
599	h	(m)	Emission height (after buoyant rise)
600	k	(-)	Topographic forcing factor
601	PBL	(m)	Planetary Boundary Layer height
602	RH	(%)	Relative humidity
603	S	(-)	Stability class
604	T	(°C)	Temperature
605	u	(m/s)	Wind speed
606	x	(m)	Plume frame of reference transverse coordinate
607	y	(m)	Plume frame of reference downwind coordinate
608	z	(m)	Plume frame of reference vertical coordinate (altitude)
609	$\alpha, \beta, \gamma, \delta, \epsilon, \psi$	(-)	Transect labels
610	σ_y	(m)	Dispersion coefficient in the y direction
611	σ_z	(m)	Dispersion coefficient in the z direction

612

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