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Supplementary Materials for

Satellite-based survey of extreme methane emissions in the Permian basin

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Text S1. Assessment of uncertainties in methane retrieval

Methane retrievals from imaging spectroscopy data can present systematic and random errors. We have performed a sensitivity analysis based on end-to-end simulations to assess retrieval errors for the conditions of our study. This comprises simulations of the at-sensor radiance for a $1.5 \times 1.5\,\mathrm{km}^2$ area in the Permian Basin with a sun zenith angle of 45° and methane plumes with flux rates of either 500 or 1000 kg/h. A 30-m pixel and the actual spectral response and signal-to-noise ratio of the GF5-AHSI, ZY1-AHSI and PRISMA spectrometers are considered in the simulations. The resulting top-of-atmosphere radiance images have been processed with the same matched-filter methane retrieval scheme that we applied to our real data (see Materials and Methods in the Main Text).

Results from this sensitivity analysis are presented in Figs. S5 and S6. A first impression of the resulting methane concentration enhancement maps (ΔXCH_4) for the simulated Permian area and plumes from 500 and 1000 kg/h sources is provided in Fig. S5. The plumes are visible for GF5-AHSI for both 500 and 1000 kg/h intensities, whereas the 500 kg/h plume is hardly detectable for ZY1-AHSI and PRISMA because of the lower signal-to-noise ratio and/or spectral resolution of these instruments with respect to GF5-AHSI.

Retrieval noise and potential biases are further evaluated in Fig. S6. The impact of retrieval noise for each instrument is indicated by the probability distribution functions generated by running the retrieval over a simulated image devoid of methane plumes (flux rate equal to 0 kg/h, Fig. S6 top row). The spread of ΔXCH_4 values responds to the retrieval sensitivity to instrumental noise and to per-pixel variations in surface albedo within the Permian area used for the simulations. The very different sensitivity to methane enhacements of the three instruments is again clear. We take the σ values of the fitted Gaussian function as typical ΔXCH_4 retrieval 1-σ (random) errors (63, 101 and 149 ppb for GF5-AHSI, ZY1-AHSI and PRISMA, respectively).

We do not observe systematic errors for any of the three instruments, either from the maps in Fig. S5 or from the scatter plots in Fig. S6 for the 500 and 1000 kg/hr sources, which suggests that the retrieval is not intrinsically biased. On the other hand, we acknowledge that instrument radiometric or spectral calibration errors could introduce systematic errors in the retrieval. However, it must be remarked that we use scene-based methods to characterize the instrument spectral response prior to the retrieval, and that our spectroscopic techniques rely on changes of the fractional depth of the methane absorption features and are therefore highly robust to absolute radiometric calibration errors.

Text S2. Verification of emission rate estimates using large eddy simulations

We used the Weather Research Forecast model version 3.9.1 coupled with Chemistry in Large Eddy Simulation mode (WRF-Chem-LES), coded for passive tracers by T. Lauvaux (*43*), to provide independent estimates of emission rates (Q) for several plumes (designated k and l from GF5-AHSI, and x from ZY1 AHSI). The model was coupled to 4-D meteorological fields from NOAA's High Resolution Rapid Refresh (HRRR) model, at the times and locations of the observed plumes. HRRR has spatial resolution of 3 km $\times$ 3 km, much finer than the 25 $\times$ 25 km resolution of the GEOS-FP model used for the IME-based estimations of Q in our work (see Materials and Methods in the Main Text). Both HRRR and GEOS-FP are updated hourly. Our WRF-Chem-LES/HRRR model domain was 8 km$\times$8 km (grid cell 111 m$\times$111 m), and model plumes were interpolated onto the satellite pixels.

In each model run, we assumed a nominal Q of 988 kg/hr. Emissions were scaled by matching the total mass of excess CH_4 in equal areas as follows: the area of each observed plume was defined objectively using the "contourLines" function of R to determine the contour enclosing the threshold for detection of ΔXCH_4 (= 0.045 ppm, i.e. 2.5% of total XCH_4, based on the variance of the retrievals of the satellite images) (see Fig. S8). The local background was defined within 1 km of the emission source. We then computed a scale factor to best match the area-integrated ΔXCH_4 of the observed plume (subtracting the local background) with the area-integrated ΔXCH_4 of the modeled plume (in equal areas). Results were insensitive to the choice of threshold due to the sharp edges of the plumes.

As shown in Fig. S8, the WRF-Chem-LES/HRRR model produces realistic plumes with distributions of ΔXCH_4 closely aligning between model and observations. The resulting Q estimates do not use any of the analysis of the IME/GEOS-FP in Table S1. The independence of these two approaches provides a rigorous test of the IME estimates in the Main Text, including the spatial form of the identified plumes and the uncertainties associated with errors in meteorological inputs and model structure. Confidence intervals for the WRF-Chem-LES/HRRR estimates were obtained from the t-statistic of seven realizations obtained every 5 minutes during the simulation, starting from 15 minutes before and ending 15 minutes after the satellite overpass.

The IME-based model as described in the Materials and Methods section of the Main Text was applied to the simulated plumes to check the consistency betweeen the two models. The impact of wind speed information on the estimated flux rates was also evaluated. The IME-based method was applied to both real and simulated data, and was contrained by either GEOS-FP or HRRR wind products. The comparison of the Q obtained from the processing of real data with the IME-based method and the two different wind products is used to evaluate the impact of wind speed on IME-based Q estimates, whereas the comparison of the two modeling methods with the same HRRR wind constraint is helpful for the assessment of intrinsic model differences.

A summary of results is presented in Table S2. It can be seen that the Q obtained with the WRF-

Chem-LES/HRRR simulations for observed plumes k and l is lower by about 50% than the Q estimated using our processing chain consisting in the IME-based method and the GEOS-FP wind information (see Materials and Methods), whereas plume x was higher by 50% (first and forth Q columns in Table S2). Wind speeds at the source locations appear to be one of the major contributors to the differences between estimates from WRF-Chem-LES/HRRR and IME/GEOS-FP. We examined HRRR and GEOS-FP winds at a nearby airport station (Winkler, TX). On 2020-02-08, HRRR winds and Winkler observations were both lower than GEOS-FP at the plume sites at the overpass time (20Z), contributing to the difference in estimated emissions in Table S2. A similar pattern also existed on 2019-11-01, at 18Z. When compared to the reported data from the nearby airport, HRRR winds were closer to the observations. However, because the winds in both WRF-Chem-LES/HRRR and IME/GEOS-FP are model products, we cannot know if HRRR data are more accurate than GEOS-FP in general.

We further evaluate the impact of wind speed on IME-based Q estimates and observe that the differences between GEOS-FP and HRRR wind speed data in the IME-based estimates can lead to differences up to 40% (first and second Q columns in Table S2), which is within the precision errors estimated for our Q calculations. On the other hand, the comparison of the two modeling methods (IME-based and WRF-Chem-LES) for the same HRRR wind information (third and forth Q column in Table S2) shows that there are also strong uncertainties associated to the particular Q estimation method. Intrinsic model uncertainties can have an impact as high as that from the winds. IME-based Q estimates are in fact very similar for real and simulated data irrespective of the wind.

The results obtained from this modeling exercise verify the very large emission sources reported in this study, with central values for the estimated rates lying just outside the estimated confidence intervals for the IME/GEOS-FP approach as indicated in Table S2. This analysis also confirms that the precision errors of up to 40% derived from the propagation of wind speed uncertainties are reliable. However, it also shows that potential structural model errors can be an important uncertainty contribution. More WRF-Chem-LES/HRRR simulations would be necessary to extract quantitative conclusions of the magnitude and sign of the contribution of model uncertainty to the total error budget.

Text S3. Robustness of confidence intervals in integrated emission rates

From the analysis of the 19 plumes detected in the GF5-AHSI acquisitions from 8-Feb-2020, we obtain an integrated emission rate of 0.28 Tg a^{-1} with a 0.20–0.35 Tg a^{-1} 95% confidence interval (CI). These are calculated through nonparametric bootstrapping of the single emission rates from each of the 19 plumes in our sample.

Because of the small size of our sample, we evaluated the robustness of the estimated total emission rate and CI. We used a subset of the Four Corners plume data set from Frankenberg et al. (*14*) to simulate a realistic distribution of 166 plumes. The shape of the Four Corners Q distribution is scaled to have a similar mean, variation range and coefficient of variation (standard deviation over mean) than our 19-plume Permian data set from 8 February 2020. The result is a distribution of 166 plumes with a realistic non-Gaussian shape and the range of values of our Permian data set. We applied the bootstrapping to 50 independent subsets of the simulated distribution. Each subset consisted of 19 plumes extracted randomly with replacement.

The result of this exercise is presented in Fig. S14. It shows the resulting total emission rate and CI for each of the 50 independent 19-plume subsets. The numbers in the legend indicate the mean and standard deviation calculated for the total emission and its CI from all 50 plumes. We obtain a mean total emission of 0.29 Tg a^{-1}, with a mean 95% CI of [0.22, 0.37] Tg a^{-1}. These values are close to the results obtained from our real Permian plumes, which suggests the experiment is realistic. The relative variability (standard deviation over mean) is 11% for the total emission and for the upper value of the CI, and 13% for the lower value, which can be understood as a rough estimate of the 1-sigma uncertainties that we can expect from the use of a small subset of plumes to represent a larger plume population.

Table S1: Summary of the detected methane plumes in the Permian Basin using satellite imaging spectroscopy data. *Figure Code* refers to the figure panel where the plume is shown, either in Fig. 1 or Fig. S10, Q is the estimated emission flux rate, and $\sigma(Q)$ its 1-σ precision error.

Mission	Figure Code	Acquisition date	Latitude (deg)	Longitude (deg)	Q (kg/h)	σ (Q) (kg/h)	Type of facility	Start of operation
GF5	F1.a; FS10.a	08/02/2020	33.082	-104.389	3590	1220	Unknown	NA
	FS10.b	08/02/2020	32.604	-104.249	977	340	Tank battery	2007
	FS10.c	08/02/2020	31.999	-104.125	743	199	Compressor station	2013
	FS10.d	08/02/2020	32.069	-104.026	2177	574	Unknown	NA
	FS10.e	08/02/2020	32.149	-103.995	967	281	Compressor station	2016
	F1.b; FS10.f	08/02/2020	32.259	-103.974	2119	608	Flaring	2018
	FS10.g	08/02/2020	31.659	-103.543	1645	508	Flaring	2018
	FS10.h	08/02/2020	31.640	-104.038	560	151	Compressor station	2018
	FS10.i	08/02/2020	31.710	-103.766	1880	500	Flaring	2018
	FS10.j	08/02/2020	31.664	-103.891	1145	308	Compressor station	2014
	F1.e; FS10.k	08/02/2020	31.752	-103.864	1626	433	Tank battery	2020
	F1.h; FS10.l	08/02/2020	31.811	-103.536	2911	902	Compressor station	2018
	FS10.m	08/02/2020	31.216	-103.341	1017	231	Tank battery	2019
	FS10.n	08/02/2020	31.185	-103.561	522	121	Tank battery	2018
	F1.f; FS10.o	08/02/2020	31.369	-103.632	4385	1296	Compressor station	2019
	FS10.p	08/02/2020	31.349	-103.661	1850	548	Flaring	2019
	FS10.q	08/02/2020	31.378	-103.482	892	211	Compressor station	2018
	FS10.r	08/02/2020	31.400	-103.431	990	231	Compressor station	2018
	FS10.s	08/02/2020	31.522	-103.463	1493	349	Compressor station	1996
	FS10.t	15/05/2019	31.976	-103.629	1340	522	Tank battery	2016
	FS10.u	15/05/2019	31.660	-103.537	1773	675	Wellhead	2007
	FS10.v	15/05/2019	31.688	-103.562	2280	865	Wellhead	2019
	FS10.w	15/05/2019	31.645	-103.938	1633	581	Compressor station	2017
ZY1	FS10.x	01/11/2019	32.276	-103.789	2119	832	Compressor station	2019
	F1.j; FS10.y	01/11/2019	32.268	-103.437	5472	2159	Compressor station	2017
	FS10.z	01/11/2019	32.007	-103.824	1998	789	Flaring	2018
	FS10.aa	01/11/2019	31.995	-103.592	2372	966	Compressor station	2016
	FS10.ab	01/11/2019	32.167	-103.648	1525	602	Compressor station	2018
	F1.d; FS10.ac	01/11/2019	31.766	-104.040	2636	1120	Flaring	2019
	FS10.ad	29/12/2019	32.021	-103.278	2350	922	Flaring	2017
	FS10.ae	29/12/2019	31.983	-103.426	3139	1260	Compressor station	2017
	F1.g; FS10.af	29/12/2019	31.540	-103.309	5952	2556	Compressor station	2012
	F1.c; FS10.ag	11/08/2020	31.876	-104.160	18492	6570	Unknown	NA
PRS	F1.i; FS10.ah	21/04/2020	32.057	-103.533	2842	1082	Compressor station	2018
	F1.d; FS10.ai	12/02/2020	31.745	-104.065	4298	1885	Tank battery	2017
	FS10.aj	07/06/2020	32.680	-103.867	1221	515	Tank battery	2019
	FS10.ak	06/07/2020	32.205	-103.718	528	165	Tank battery	2019

Table S2: Summary of emission rate estimates (Q) from the IME-based method used in this study and the alternative WRF-Chem-LES/HRRR simulations described in Text S2 for three of the observed emissions. The IME-based method is applied to both real and simulated data, and is contrained by either GEOS-FP or HRRR wind products. ASOS KINK refers to the wind information from the Automated Surface Observing System at the Winkler County Airport.

Mission	Figure code	Real data		Simulation		GEOS-FP Wind (m/s)	HRRR Wind (m/s)	ASOS at KINK Wind (m/s)
		IME/GEOS-FP Q (kg/h)	IME/HRRR Q (kg/h)	IME/HRRR Q (kg/h)	WRF-Chem-LES/HRRR Q (kg/h) [95% CI]			
GF5	F1.e; FS10.k	1626 ± 433	1364 ± 307	1588 ± 354	690 [660, 840]	1.47 @ 19:30 UTC	0.68 @ 19:00 UTC	0.00 @ 19:00 UTC
							1.03 @ 20:00 UTC	1.20 @ 20:00 UTC
							1.98 @ 21:00 UTC	2.91 @ 21:00 UTC
	F1.h; FS10.l	2911 ± 902	2267 ± 583	2497 ± 642	1420 [1360, 1450]	2.14 @ 19:30 UTC	1.37 @ 19:00 UTC	0.00 @ 19:00 UTC
							1.38 @ 20:00 UTC	1.20 @ 20:00 UTC
							1.34 @ 21:00 UTC	2.91 @ 21:00 UTC
ZY1	FS10.x	2119 ± 832	1314 ± 420	2146 ± 683	3180 [2880, 3460]	4.45 @ 17:30 UTC	1.14 @ 18:00 UTC	0.00 @ 19:00 UTC
							2.27 @ 19:00 UTC	4.12 @ 20:00 UTC
							3.22 @ 20:00 UTC	4.63 @ 21:00 UTC

Figure S1: Sensitivity of satellite imaging spectroscopy measurements to methane column enhancements. Left, simulated GF5-AHSI spectra for different methane levels (500 ppb enhacement); right, unit absorption spectrum used for enhancement retrieval with the matched-filter approach.

Figure S2: Spatial coverage of the spaceborne imaging spectroscopy data used in this work. Most of the images used in this study were taken on 4 different days between May 2019 and August 2020 (15 May 2019 and 8 February 2020 for GF-5 AHSI, and 1 November 2019 and 29 December 2019 for ZY1 AHSI).

Figure S3: Illustration of the process for the extraction of methane plumes from raw ΔXCH_4 maps. An example is shown in the top-left panel. The top-right panel shows the enhancement map after masking out pixels with ΔXCH_4 below 200 ppm·m, the bottom-left panel shows the mask manually delineated, and the bottom-right panel shows the final extent of the plume.

Figure S4: Relationship between 10-m wind speed (U_{10}) and effective wind speed (U_{eff}) derived for the typical measurement uncertainty and plume detection limit of the instruments used in this work.

Figure S5: Methane retrieval results from end-to-end simulations optimized for the Permian Basin and the three space-based instruments used in this study (500 kg/h emission case on the left column, and 1000 kg/h case on the right).

Figure S6: Same data as in Fig. S5, but including the histogram of the retrieved ΔXCH_4 in the case of no emission (top row) and the comparison between input and retrieved methane concentrations for the 500 and 1000 kg/h cases (center and bottom rows). The dash line in the scatter plots represents the 1:1 line, and the red line the fitted linear model.

Figure S7: Flux rate values and precision errors estimated from the 37 plumes detected in this study. The flux rates including their precision error are shown in the lower panel (similar to Fig. 2 of the main text). The relative precision errors (error normalized by flux rate) are represented in the top panel.

Figure S8: Observed (left) and modelled (right) plumes of (a) *plume k* on 2020-02-08 and (b) *plume x* on 2019-11-01. The modelled plume was generated by using WRF-Chem-LES with topography and one-way coupling to full HRRR meteorology. We used the "contourLines" function in R to identify the enclosing area with a detection threshold of ΔXCH4 (threshold = 0.045, ppm, i.e. 2.5% of total XCH4), defining the dashed black line in the main image (red box). The selected plume is shown in the solid white box at the bottom right corner. The red sun-cross symbols indicate the source locations.

Figure S9: Satellite-detected methane emissions over the Permian basin colocated with (left) the bottom-up emission inventory from the US Environmental Protection Agency (*28*) updated to account for 2020 infrastructure, and (right) top-down emission estimates from the inversion of TROPOMI observations using Bayesian atmospheric inverse modeling (data from Zhang et al. (*8*)).

Figure S10: Visual representation of the detected methane plumes in the Permian Basin using satellite imaging spectroscopy data (see Table S1).

Figure S10: (Cont.)

Figure S11: Comparison of the methane enhancement map derived from a ZY1-AHSI aquisition on 11 August 2020 with independent expressions of the surface composition. The *mineralogy* image is built as an RGB image with the first three principal components of a PCA decomposition using 2100-2400 nm bands where different minerals and surface components present characteristics spectral features. Greenish tones likely indicate a higher presence of carbonates.

Figure S12: Maps of column averaged dry air mole fraction of methane (XCH_4) derived from TROPOMI data over the area where the massive methane enhancement was detected on 11 August 2020 (marked with a black cross). No map is shown for 11 August 2020 because the area was covered by clouds during the TROPOMI overpass.

Figure S13: Examples of methane emission plumes from the same infrastructure detected in both our satellite data and airborne AVIRIS-NG imaging spectroscopy data.

Figure S14: Bootstrapping test for a reduced sample of 19 plumes. (Top) Set of 166 simulated plumes matching the mean, range and coefficient of variation of our Permian 8-February-2020 data set. (Bottom) Bootstrapping results obtained from 50 independent 19-plume subsets out of a 166-element population. The legend gives the mean and the standard deviation for the total value and the 95% confidence interval (CI) from all 50 cases.

Figure S15: Illustration of the visual attribution of detected methane plumes to particular infrastructure elements. For each of the three sub-figures, the area in the red rectangles is zoomed in in the lower part of the panel. The grey image on the top-left panel shows the high radiance measured in the 2300 nm spectral region at the emission source due to the high temperature of the flare. From left to right, panels correspond to codes F1.b, FS8.aa and FS8.t in Table S1. See Fig. S10 for the corresponding colorbar.