



U-Plume: Automated algorithm for plume detection and source quantification by satellite point-source imagers

Jack H. Bruno^{1,2}, Dylan Jervis², Daniel J. Varon¹, Daniel J. Jacob¹

5 ¹Earth And Planetary Sciences, Harvard University, Cambridge, MA, 02138, USA

²GHGSat Inc, Montreal, Quebec, H2W1Y5, Canada

Correspondence to: Jack H. Bruno (jackbruno@g.harvard.edu)

Abstract. Current methods for detecting atmospheric plumes and inferring point source rates from high-resolution satellite imagery are labor intensive and not scalable to the growing satellite dataset available for methane point sources. Here we present a two-step algorithm called U-Plume for automated detection and quantification of point sources from satellite imagery. The first step delivers plume detection and delineation (masking) with a machine learning U-Net architecture for image segmentation. The second step quantifies point source rate from the masked plume using wind speed information and either a convolution neural network (CNN) or a physics-based Integrated Mass Enhancement (IME) method. The algorithm can process 62 128×128 images per second on a single core. We train the algorithm with large-eddy simulations of methane plumes superimposed on noisy and variable methane background scenes from the GHGSat-C1 satellite instrument. We introduce the concept of point source observability $O_{ps} = Q/(UW\Delta B)$ as a single dimensionless number to predict plume detectability and source rate quantification error from an instrument as a function of source rate Q , wind speed U , instrument pixel size W , and instrument-dependent background noise ΔB . We show that O_{ps} can powerfully diagnose the ability of an imaging instrument to observe point sources of a certain magnitude under given conditions. U-Plume successfully detects and masks plumes from sources as small as 100 kg h⁻¹ over surfaces with low background noise and succeeds for larger point sources over surfaces with substantial background noise. We find that the IME method for source quantification is unbiased over the full range of source rates while the CNN method is biased toward the mean of its training range. The total error in source rate quantification is dominated by wind speed at low wind speeds and by the masking algorithm at high wind speeds. A wind speed of 2-4 m s⁻¹ is optimal for detection and quantification of point sources from satellite data.

25

Keywords: Methane, Point Sources, Satellites, Machine Learning, Image Segmentation

1 Introduction

A number of satellite instruments can now detect and image methane column plumes with spatial resolution finer than 50 m by solar backscatter in the shortwave infrared (SWIR), enabling quantification of large point sources from individual facilities (Jacob et al., 2022). As the satellite observing system expands for both methane and other gases, there is a growing need for efficient methods of detecting and quantifying these point sources by automated processing of vast amounts of data. Here we

30



present the U-Plume algorithm, a generalized machine-learning method to address this need, and we apply it to methane observations from GHGSat (Jervis et al., 2021).

35 Several methods have been proposed for inferring point source rates from satellite imagery of atmospheric pollution plumes, including for methane (Varon et al. 2018), CO₂ (Nassar et al. 2017), NO₂ (Valin et al. 2013; De Foy et al. 2015; Beirle et al. 2021), CO (Pommier et al. 2013), SO₂ (Fioletov et al. 2015; McLinden et al. 2016), and NH₃ (Clarisse et al. 2019; Dammers et al. 2019; Noppen et al. 2023). Gaussian plume inversion (Bovensmann et al., 2010; Krings et al., 2011, 2013) and mass
40 plumes (>10 km) but they fail when applied to sub-km plumes due to stochastic turbulence that leads to non-Gaussian behavior and dominance of eddy flow (Varon et al., 2018). Temporal averaging of plumes over multiple satellite passes with wind rotation has been used extensively for large plumes from well-identified point sources to decrease noise and enhance Gaussian behavior (Pommier et al. 2013; Fioletov 2015; McLinden et al. 2016; Varon et al., 2020; Massakers et al. 2022), but is difficult to implement for methane plumes that are typically smaller and intermittent (Frankenberg et al., 2016; Cusworth et al., 2021).

45

Two methods that have shown success in estimating emissions from high-resolution instantaneous plume imagery are the Integrated Mass Enhancement (IME) and Cross-Sectional Flux (CSF) methods (Krings et al. 2011, 2013; Frankenberg et al. 2016; Varon et al. 2018). The IME method relates the total observed plume mass to a source rate, using information from the plume size and the local wind speed. The CSF method integrates concentrations over plume cross-sections perpendicular to
50 the wind direction and multiplies them by the local wind speed to infer a source rate. Both methods require the plume to be identified and masked (i.e., delineated) within the image.

Detection and masking of plumes in satellite scenes has generally been done by human analysts (Guanter et al., 2021) but this is not practical operationally. Simple statistical thresholding approaches combined with adjacency criteria have been developed
55 to detect methane enhancements above background for plume masking (Varon et al., 2019; Duren et al. 2019) but these are vulnerable to retrieval artifacts, particularly from surface features mistakenly identified as methane plumes (Cusworth et al., 2019).

Machine learning is a promising avenue for automating plume detection and inference of point source emissions.
60 Jongaramrungruang et al. (2022) proposed a Convolutional Neural Network (CNN) to estimate source rates directly from aerial AVIRIS-NG methane imagery. Their method (called MethaNet) provides source rate estimates based solely on methane column retrieval fields, forgoing the use of external information on wind speed by exploiting wind information contained in the morphology of the plumes (Jongaramrungruang et al., 2019). Training and testing of MethaNet has been done on aircraft imagery with relatively clean backgrounds and high pixel resolution (3 m), but to our knowledge it has not been applied to
65 satellite imagery which is coarser and more vulnerable to surface artifacts. MethaNet does not produce a plume mask (outline



of plume boundaries), but such a mask offers important visual information and can help identify artifacts. Joyce et al. (2023) used a U-Net architecture to mask methane plumes in PRISMA satellite imagery directly from radiances and again without wind speed information. Separate networks were then used for inferring methane column concentration and estimating emission rates. In both MethaNet and the Joyce et al. (2023) approach there is a bias towards the training mean in the final source rate estimates, resulting in overestimate of low emitting plumes and underestimate of high emitting plumes. This is a common issue in machine learning applications.

Here we perform binary segmentation of methane column imagery from GHGSat using a U-Net neural network architecture to produce plume masks, and we then use these masks together with wind speed information to infer point source rates either with a CNN or with the physics-based IME method. We use wind speed information because some is always available, either from local measurements or from regional/global reanalysis datasets. The U-Net architecture (Ronneberger et al. 2015) has previously demonstrated to be effective in feature recognition by binary image segmentation from satellite imagery (Joyce et al. 2023), avoiding the false positives present in more traditional methods reliant on thresholding (Rezvanbehbahani et al. 2020). Combining the U-Net architecture to detect plumes in column enhancement with subsequent steps to infer point source rates forms an end-to-end algorithm that we call U-Plume.

2 Methods

We present here the U-Plume algorithm for identifying point source plumes in satellite imagery of methane concentrations and inferring point source rates. The algorithm has two components: (1) a U-Net to detect plumes by binary segmentation of the pixels in the satellite scene (0 = background, 1 = plume), producing a plume mask; (2) two alternative CNN and IME approaches for inferring source rates from the plume mask. We demonstrate U-Plume on the GHGSat-C1 instrument for methane, but the architecture and training process presented here are applicable to any satellite point source imagers for any species.

GHGSat-C1 is the first operational instrument launched in 2020 by GHGSat Inc., following the demonstration instrument GHGSat-D launched in 2016 (Jervis et al., 2021). The instrument is a shortwave interferometer with an observation domain of $\sim 12 \times 12 \text{ km}^2$ at $25 \times 25 \text{ m}^2$ pixel resolution. Retrieval of the backscattered solar spectrum at the $1.65 \text{ }\mu\text{m}$ methane absorption band yields an estimated methane column mass enhancement over background reported as mol m^{-2} with 1-2% estimated precision. The instrument is in polar sun-synchronous orbit with observation at $\sim 9:30$ am local time. Subsequently launched GHGSat-C2-C8 instruments have less background noise than -C1. Our results can be extended to C2-C8 and any other instruments using the background noise metrics presented below.

Our first step is to create a training data set of plume-containing satellite images in which synthetic instantaneous plumes of known source rates are superimposed on actual plume-free images. Following Varon et al. (2018) and Jongaramrungruang et



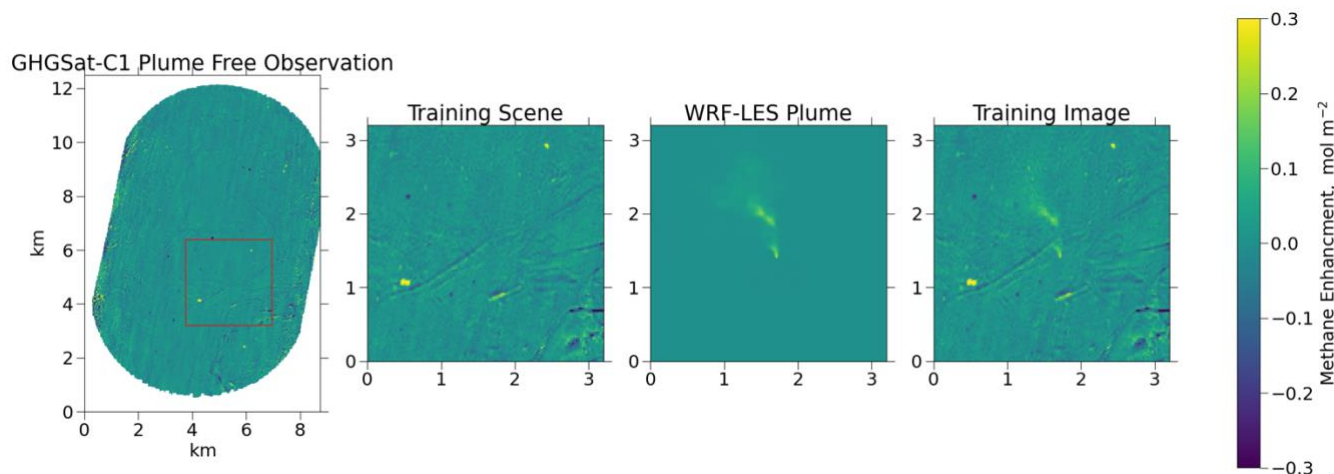
100 al. (2019), we use the Weather Research and Forecasting Model Large Eddy Simulation (WRF-LES) to create a diverse plume
dataset of atmospheric methane concentration enhancements where the relationship between source rate and plume
concentrations is known. Point source methane emission and atmospheric transport are simulated on a $25 \times 25 \text{ m}^2$ horizontal
and 15-m vertical grid over a $9 \times 9 \times 2.4 \text{ km}^3$ domain, with the point-source emitting at the surface $5/6$ from the downwind edge
of the domain. We conduct 4 simulations for different meteorological conditions, each run for 3 hours with the first hour used
as spin-up, resulting in 2 hours of usable plume images per simulation. Time steps for WRF-LES integration are $1/4$ second
105 and instantaneous plumes are sampled every 30 seconds. Mean wind speeds for the simulations are $3\text{-}9 \text{ m s}^{-1}$ with sensible heat
fluxes of $100\text{-}300 \text{ W m}^{-2}$ and mixed layer depths of $500\text{-}2000 \text{ m}$. This is the same ensemble as used by Varon et al (2021).

To create an effective neural network, the training imagery must be as close as possible to the real observations that the model
will be applied to. Previous work by Varon et al. (2018) using WRF-LES to simulate synthetic plumes superimposed these
110 plumes on a white-noise background to generate a training data set, but variable surface albedo and terrain can lead to
heterogenous noise fields with complex structure. To create realistic noise for our training images we start from a set of actual
GHGSat-C1 observations of plume-free scenes and add the methane column enhancements from the WRF-LES simulation.
We use the standard deviation of the pixel enhancements in the plume-free scene ($\Delta B, \text{kg m}^{-2}$) as measure of background
noise:

115

$$\Delta B = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n}} \quad (1)$$

Here n is the number of pixels in the image, x_i is the column concentration for individual pixel i , and \bar{x} is the mean column
concentration in the scene. When discussing ΔB we express it as a percentage of the global mean background concentrations
120 (taken as $x_b = 0.011 \text{ kg m}^{-2}$; Jervis et al., 2021). We use 28 $12 \times 12 \text{ km}^2$ GHGSat-C1 plume-free observations corresponding to
a variety of surface types. Scenes with $\Delta B < 5\%$ correspond to homogenous bright surfaces including arid and grassland
terrain. Scenes with $5\% < \Delta B < 10\%$ correspond to moderately heterogeneous surfaces. Scenes with $\Delta B > 10\%$ correspond
to very heterogeneous or dark surfaces including forests, wetlands, and urban areas. Values of ΔB are instrument dependent.
The more recent GHGSat-C2 and beyond instruments have $\Delta B < 2\%$ and across all scenes and observing conditions (Ramier,
125 2022). On the other hand, hyper/multi-spectral land surface mappers can have background noise exceeding 10% (Cusworth et
al., 2019; Varon et al., 2021).



130 **Figure 1: Sample generation of U-Plume training imagery.** The first panel shows a sample plume-free observation of methane column concentration enhancements observed by GHGSat-C1. Panel 2 is a 128×128-pixel scene randomly selected from the full observation domain. Panel 3 shows a sample WRF-LES instantaneous plume for a source rate of 2000 kg h⁻¹ (we choose a large plume here for easy visualization). Panel 4 shows the result of adding panels 2 and 3 to form a training image. 0.1 mol m⁻² corresponds to a dry column mixing ratio enhancement of 284 ppb.

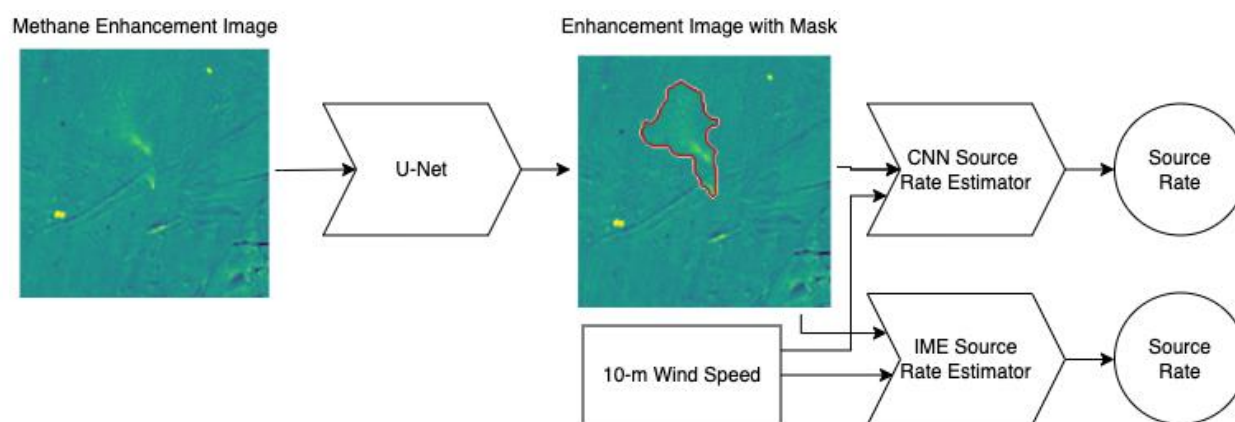
135 Fig 1 illustrates the steps for creating the synthetic plume observations used in training and testing our method. For each training image, a 128×128-pixel scene is randomly selected from a plume-free GHGSat-C1 observation. A random plume from the WRF-LES dataset is then selected, with a random rotation and translation applied to situate the plume anywhere in the scene but with a safeguard to ensure that the plume is fully contained in the scene. Since the methane enhancement in the plume is proportional to source rate, we can scale the plume randomly to correspond to a given source rate. This plume image
 140 is then added to the selected scene to create a training image. A training range of plumes emitting in the 500-2000 kg h⁻¹ is chosen to ensure that the plumes are at least partially visible in most training images. Though we want the network to be able to detect smaller source rates, it is important that the structural features being searched for are visible above noise within the training dataset. Because the U-Net recognizes structure, not just enhancement, the network trained on the 500-2000 kg h⁻¹ range is still usable outside of this range as we will see.

145

Our set of training/test images is created using 28 plume-free observations. We step the 128×128-pixel scene in 16-pixel steps to create a set of scenes. The ΔB values of these scenes range from 1% to more than 50%. We only use scenes with $\Delta B < 20\%$ to avoid training on scenes with extremely high background variability where detection of any but the largest plumes would be intractable. This filtering leaves us with a total of 6870 scenes. We then apply the random plume placement and source
 150 magnitude as described above to create 6870 simulated plume observations. The true plume mask is defined as pixels where the enhancement from the LES simulation is higher than the ΔB of the scene, which is the criterion for the pixel contributing more information than noise (Varon et al., 2018). 90% of the images are used for training and 10% are set aside for testing.



155 Fig. 2 shows the two-step process used to obtain source rate estimates from methane enhancement images. First, a U-Net
masking network is used to identify pixels in which a plume is present. The binary mask created by this network is then fed
along with the original enhancement image and external wind speed data to estimate the source rate from the identified plume.
The enhancement image with mask is preserved for visualization and as a quality control diagnostic. Processing the test dataset
of 687 images on a single 2.6 GHz Intel Core i7 CPU takes 11 seconds, corresponding to 62 images per second.



160

Figure 2: U-Plume architecture. Starting from a methane enhancement image (the sample image of fig.1), we use the U-Net machine learning algorithm to produce a plume mask (in red) of pixels containing more information than noise. All masked pixels in a single 128×128-pixel (3.2×3.2 km²) scene are assumed to originate from the same plume. We then use the original enhancement image, the mask, and local 10-m wind speed to quantify emissions using either a machine learning method or an Integrated Methane Enhancement (IME) method.

165

The U-Net neural network for plume masking (Ronneberger et al. 2015) uses an encoder-decoder framework to recognize structural features within imagery. The network receives a methane enhancement image as in Fig. 2 and classifies each pixel with a confidence level for the presence of a plume. We apply a threshold of 50% confidence to produce a binary plume mask. The main advantage of this method over traditional threshold masking is that high enhancement features that do not have plumelike shape characteristics will not be falsely captured as plumes.

170

The encoder portion of the network applies a series of convolutional filters and pooling layers to identify features of increasing complexity within the image. At the end of the encoding the image has been compressed spatially and has many channels corresponding to the various feature maps created by the convolutional filtering. By compressing the image spatially in this way, the network can recognize connections between distant features.

175



The decoder portion of the network serves to interpret these identified features as criteria for classification. An inverse
180 convolutional operator is used to expand the spatially compressed image back to the original size of the input image while
reducing the number of filters applied, which compresses the number of channels in the image. The final step of the network
uses the information gathered from the encoder-decoder process to estimate a confidence level (0-1) that each pixel is or is not
part of a plume. Output from this model for a single image is a confidence mask for plume location across the enhancement
image as shown in Figure 2. In practice, the confidence mask is generally either very close to 1 or very close to 0. Intermediate
185 values fall off very quickly at the edge of the mask.

Once the U-Net mask has been generated as the first step of our U-Plume algorithm, we infer the source rate as a second step
using as options either a CNN method or an IME method. The CNN method takes in a 3-channel input image containing the
original image, the binary mask, and 10-m wind speed. Initial testing indicated that including wind direction did not improve
190 performance. The wind speed channel is populated with a uniform 15-minute scene average value from the LES simulation.
The CNN uses a series of convolutional and pooling layers which connect to a set of fully connected layers, rather than a
decoder, to yield a scalar estimate of emissions.

The IME method follows Varon et al. (2018), in which the plume mass enhancement (IME) is combined with a parameterized
195 effective wind speed (U_{eff}) and plume length scale (L) to infer the source rate (Q , kg h^{-1}):

$$Q = \text{IME} \frac{U_{eff}}{L} \quad (2)$$

The plume length scale L is defined as the square root of the plume mask area. The effective wind speed is fitted to the 15-
200 minute averaged wind speed U_{10} at 10-m altitude using the training data set where the relationship between Q , IME, and L is
known for a given U_{10} . This yields

$$U_{eff} = 0.7 + 0.23 U_{10} \quad (3)$$

205 with U_{eff} and U_{10} in units of m s^{-1} . The intercept of 0.7 m s^{-1} arising from the fit can be physically interpreted as a minimum
turbulent diffusion for the plume at low wind speeds.

3 Dimensionless Point Source Observability Number

We introduce the concept of point source observability (O_{ps}) as a dimensionless number to determine the ability of a satellite
instrument to detect and quantify point sources. Observability is a function of source rate (Q , kg s^{-1}), wind speed (U , m s^{-1}),
210 instrument pixel resolution (W , m), and scene-dependent background noise (ΔB , kg m^{-2} , as defined by equation (1)).



The idea behind the O_{ps} concept is that the observability of point sources is determined by the signal-to-noise ratio in the plume (Varon et al., 2018). The column concentration enhancement in the plume (kg m^{-2}) scales as Q/UW (Jacob et al., 2016). The noise for a given scene (kg m^{-2}) is given by ΔB which is a scene-dependent property of the instrument that can be characterized as a function of surface type. ΔB can be viewed as the precision of the instrument accounting for the contribution from surface artifacts. The dimensionless point source observability number O_{ps} is then given by

$$O_{ps} = \frac{Q}{UW\Delta B} \quad (4)$$

and is a measure of the signal-to-noise ratio. We will use it here to interpret our results, but it can be applied more generally to any remote sensing observation of point sources.

4 Results

4.1 Plume Detection and Masking

Fig. 3 shows the relationship between source rate and U-Net masking success. The metric we use for masking success is the Jaccard score, which is the intersection of the predicted mask (A) and true mask (B) over the unity of the two:

$$J(A, B) = \frac{A \cap B}{A \cup B} \quad (5)$$

In 2% of cases no mask is produced for the image, and in 30% of cases there is no overlap between the true and predicted masks. These failures occur for high background noise ($\Delta B < 5\%$) and lower emission rates. On the other hand, Jaccard scores generally exceed 0.5 for low background noise ($\Delta B < 5\%$).

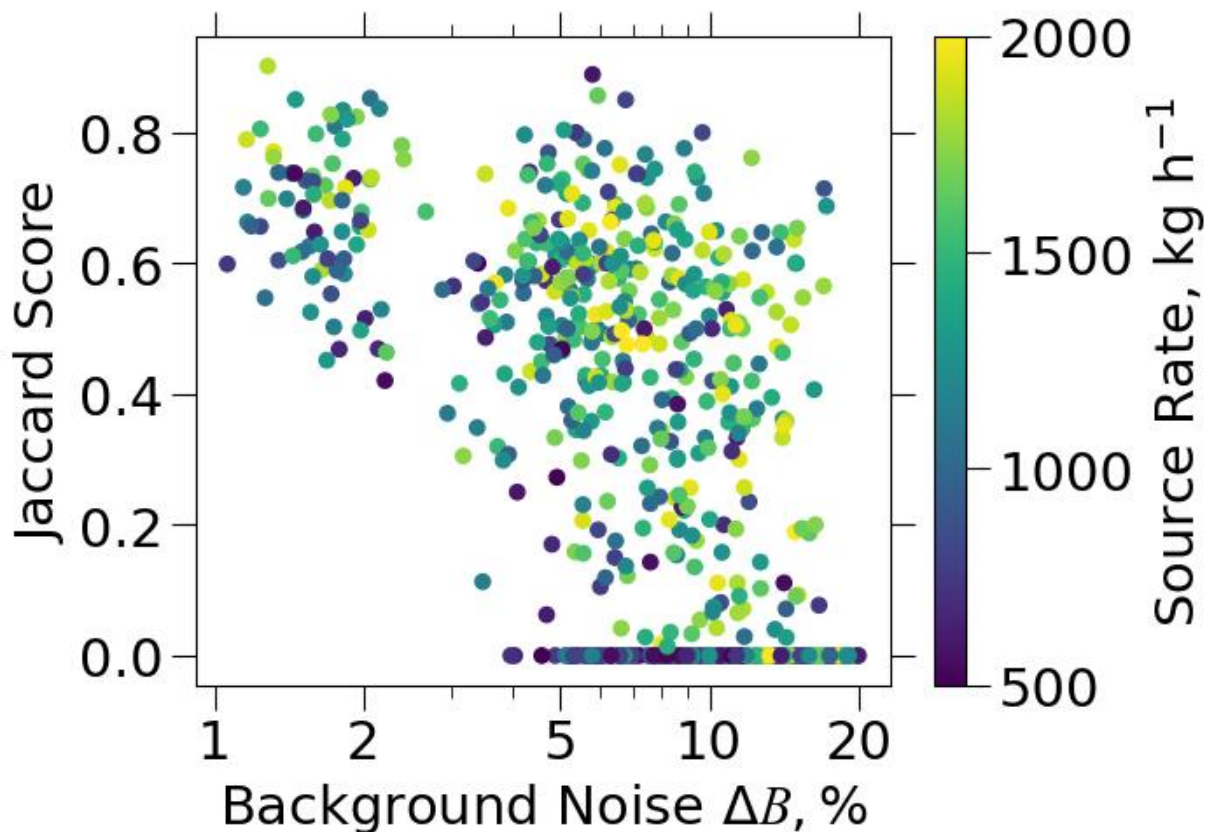
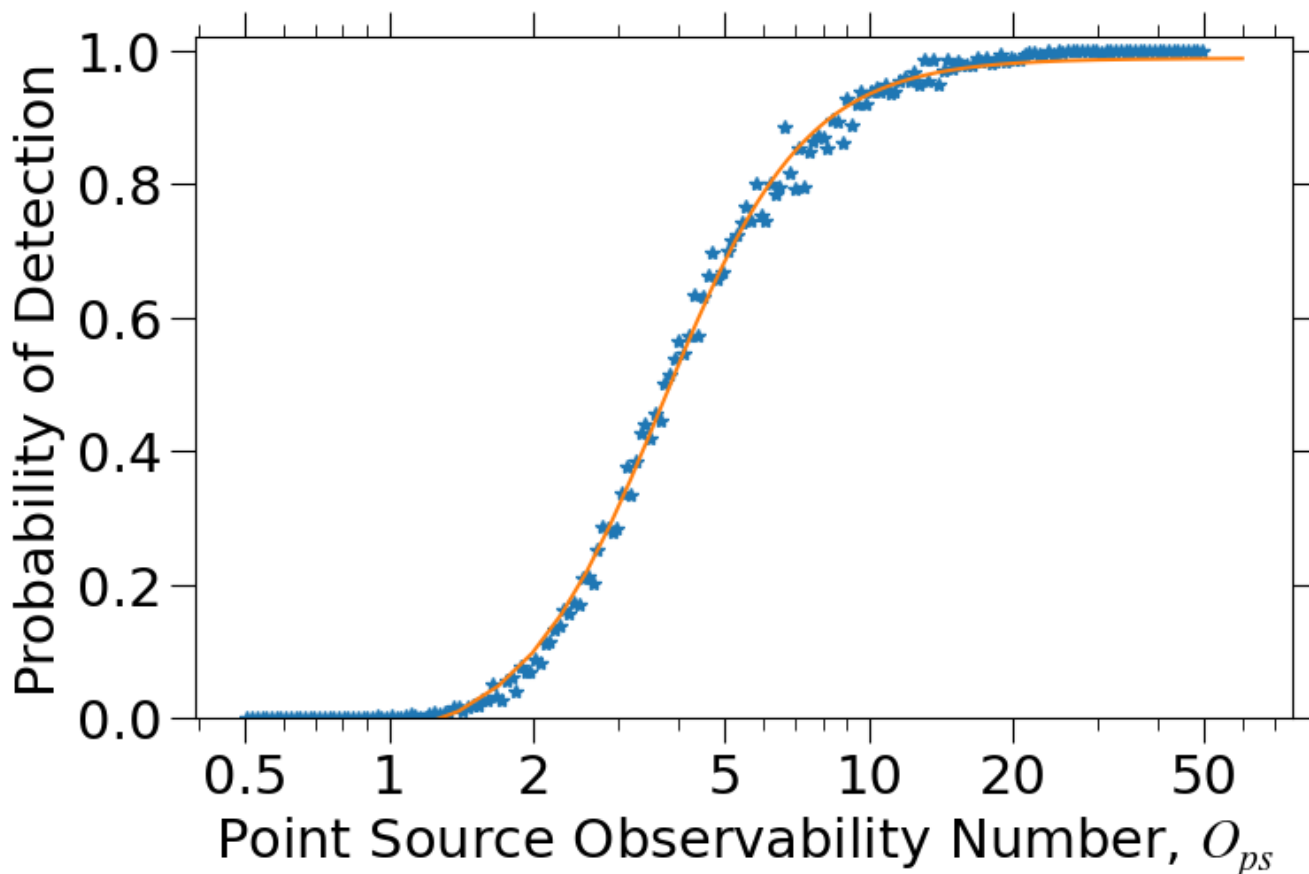


Figure 3: Ability of the U-Net machine learning algorithm to delineate (mask) plumes emitted from point sources. Masking success is measured by the Jaccard score (equation (5)) and is plotted as a function of background noise ΔB (equation (1)) for a range of point source rates from 500 to 2000 kg h^{-1} . Results are for the test set of WRF-LES plume images superimposed on noisy plume free observations from the GHG-Sat C1 satellite instrument.

We examine false positives by applying the network over the test dataset of backgrounds without plumes added. This yields 240 masks in 14% of cases (false positive detection rate). The masks produced in these false positives are generally very small, with a median size of 5 pixels. Applying a minimum 5-pixel mask size brings the false positive rate down to 6% while losing only 1.6% of the true positive detections in the test data set and removing 92% of the zero overlap masks.



245

Figure 4: Probability of detection ($J > 0.1$) for point sources in the GHGSat-C1 augmented test data set as a function of the point source observability dimensionless number O_{ps} (equation (4)). Calculation of O_{ps} uses the WRF-LES 10-m wind speed for U and the GHGSat-C1 pixel size $W = 25$ m.

250 The point source observability (O_{ps}) in equation (4) provides a scaling dimensionless number to better understand how point source detection for a given instrument relates to the combination of source rate, background noise, wind speed, and pixel size. Here we use the 10-m wind speed (U_{10}) in the calculation of O_{ps} . We create an augmented test dataset with 10 subset images from each of the 28 plume-free observations (Figure 1) and 20 emission levels for each image from 100 to 2000 kg h⁻¹ in 100 kg h⁻¹ increments. We bin images in the augmented test dataset by their O_{ps} ranging from 0.5 to 50 in 201 log-spaced bins, and
 255 for each bin with a minimum of 50 images we calculate the probability of detection as the fraction of plumes in the bin with $J > 0.1$. Figure 4 shows the relationship between the probability P of detection and O_{ps} . The relationship for $O_{ps} > 1.4$ can be tightly fit to a sigmoid function of the form:

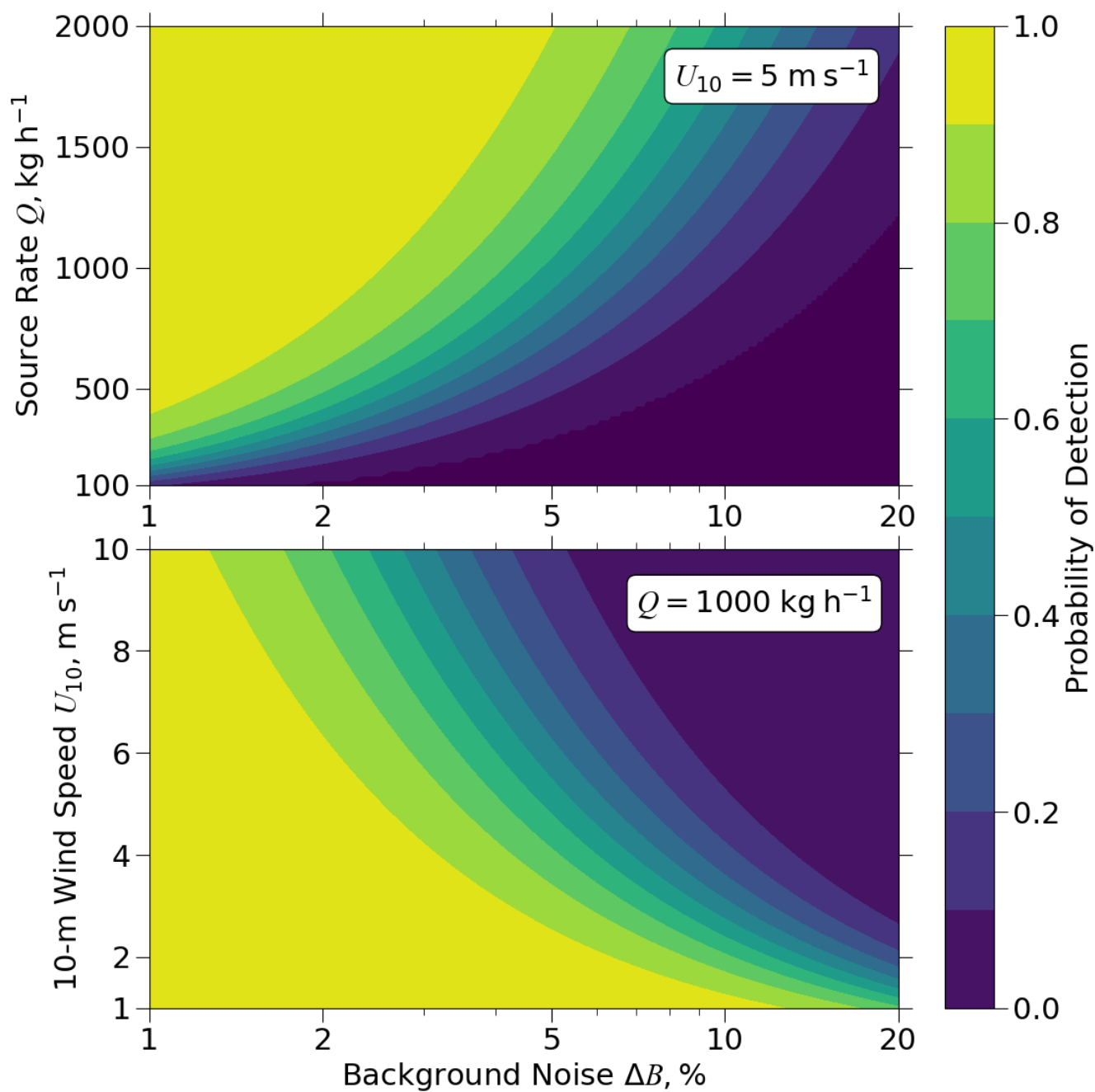
$$P = \frac{1.03}{1 + e^{-2.9(\log(O_{ps})-1.3)}} - 0.05 \quad (O_{ps} > 1.4) \quad (6)$$



260

Detection probability is 10% for $O_{ps} = 0.2$, 50% for $O_{ps} = 4$, and 90% for $O_{ps} = 8$. The transition from low detectability (<10%) to high detectability (>90%) is very sharp in O_{ps} space, demonstrating the power of the O_{ps} metric for evaluating the ability of plume imaging instrument to observe point sources. The value $O_{ps} = 4$ for the 50% detection threshold can be interpreted as a characteristic concentration enhancement $Q/4UW$ in the plume. The maximum concentration enhancement in the source pixel would be Q/UW (Jacob et al., 2016).

265



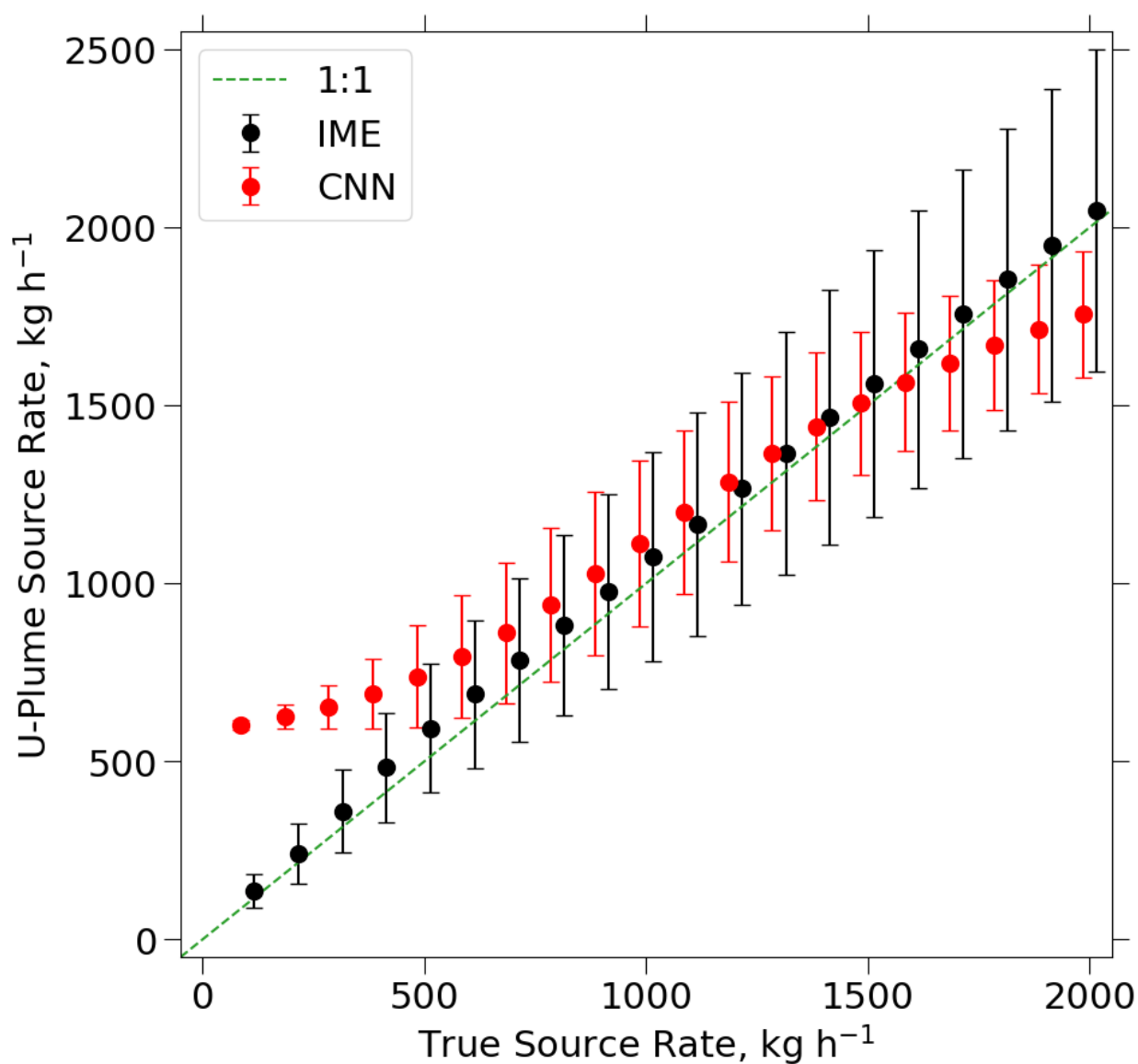
270

Figure 5: Probability of detection ($J > 0.1$) for point sources calculated using equation (6) as a function of background noise (equation (1)), source rate (top panel), and 10-m wind speed (bottom panel).



Fig. 5 shows the probability of detection calculated using equation (6) as a function of source rate, 10-m wind speed, and background noise. For low values of ΔB , the probability of detection is very sensitive to changes in Q and less sensitive to changes in U_{10} . With $\Delta B = 1\%$, 90% probability of detection is achieved for $Q > 400 \text{ kg h}^{-1}$. Conversely, for high values of ΔB the probability of detection is very sensitive to changes in U_{10} and less sensitive to changes in Q .

4.2 Source Rate Estimation





280 **Figure 6: Source rate estimates from the alternative CNN and IME methods (Figure 2) for point sources emitting in the 100-2000 kg h⁻¹ range (discrete 100 kg h⁻¹ bins) in the augmented test dataset. The methods were trained with source rates in the 500-2000 kg h⁻¹ range. Only images with Jaccard scores > 0.1 are processed. Error bars show 1 standard deviation of estimates.**

285 Fig. 6 shows the source rate estimates for the complete U-Plume workflow, starting from the plume imagery and applying either the CNN or the IME method for source rate quantification. We restrict our analysis to plumes with Jaccard score >0.1 to enable generalization to instruments with less background noise than GHGSat-C1 (such as GHGSat-C2) or to the use of improved filtering such as requiring a minimum number of plume pixels. Results are for the augmented dataset covering the 100-2000 kg h⁻¹ range but trained only over the 500-2000 kg h⁻¹ range. We assume for now no error on wind speed.

290

The CNN method has a smoothing bias where low source rates are overestimated, and high source rates are underestimated. This smoothing towards the mean is a common issue in machine learning methods and appears in the work of Jongaramrungruang et al. (2022) and Joyce et al. (2023). In addition, the CNN method is unable to extrapolate outside its training range. By contrast, the physically based IME method can successfully fit source rates all the way down to 100 kg h⁻¹ as long as the plumes are detectable. Discussion from this point forward will focus on the IME method as performing better than the CNN method over the full range of source rates. We retain the CNN method as an option in the U-Plume algorithm because it offers an alternative source rate estimate for verification purposes and because it could be improved in the future with a more extensive training dataset.

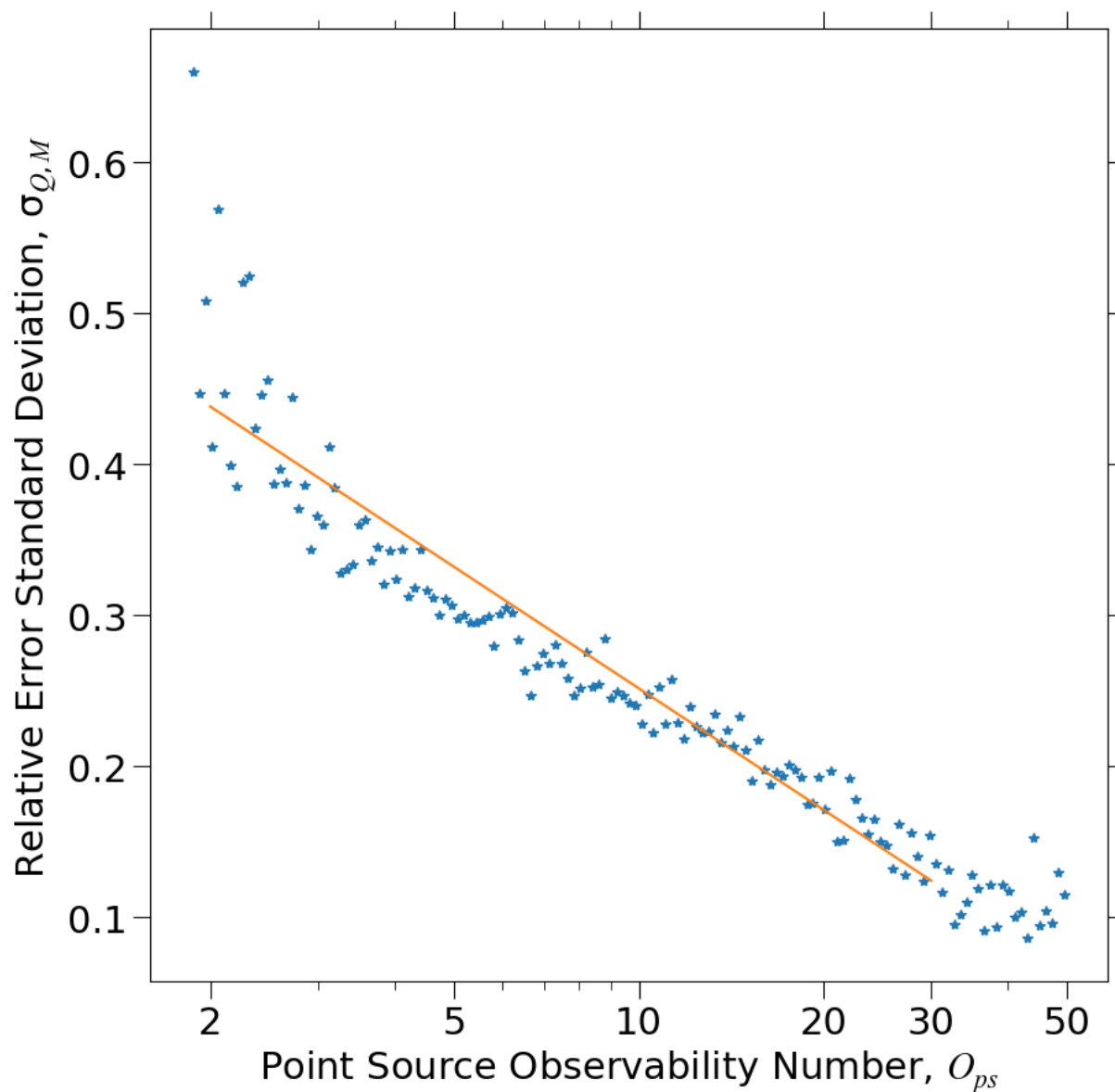
295

300 4.3 Error Analysis

The uncertainty on source rate estimates using U-Plume with the IME method can be expressed as the relative error standard deviation (σ_Q) of the U-Plume estimate versus the true value. It has two independent components: (1) error in the U-Plume algorithm, including the masking process and the IME parameterization ($\sigma_{Q,M}$); and (2) error in the 10-m wind speed ($\sigma_{Q,U}$). Here we derive expressions for $\sigma_{Q,M}$ and $\sigma_{Q,U}$ and add them in quadrature to quantify the overall error and determine the driving factors.

305

The relative error standard deviation $\sigma_{Q,M}$ from the U-Plume algorithm can be parameterized using the augmented test data set binned by point source observability O_{ps} following the approach in section 4.2 using only bins with >50 positive detections ($J > 0.1$). Figure 7 shows the relative error standard deviation plotted against O_{ps} .



310

315

Figure 7: Relative error on source rate estimation by the U-Plume algorithm. The figure shows the relative error standard deviation $\sigma_{Q,M}$ versus the point source observability dimensionless number O_{ps} (equation (4)). Errors are calculated for point sources emitting in the 100-2000 kg h⁻¹ range (discrete 100 kg h⁻¹ bins) in the augmented test dataset, not including error in wind speed (for which the error is calculated separately, see text). Errors from individual images are binned by values of their point source observability (equation (4)) for $O_{ps} = 0.5-50$ in 201 log-spaced intervals. The orange line is a reduced-major-axis (RMA) regression fit ($R^2 = 0.89$) for $\sigma_{Q,M}$ versus O_{ps} (equation (7)).

Fitting the error to $\log(O_{ps})$ yields:



320
$$\sigma_{Q,M} = \max(0.1, (0.52 - 0.12 \log(O_{ps})) \quad (O_{ps} > 2) \tag{7}$$

For values of $O_{ps} < 2$ the probability of detection is less than 10% (section 4.1). The relative error standard deviation bottoms out at 10% for highly observable plumes ($O_{ps} > 30$), reflecting irreducible error inherent to the IME method.

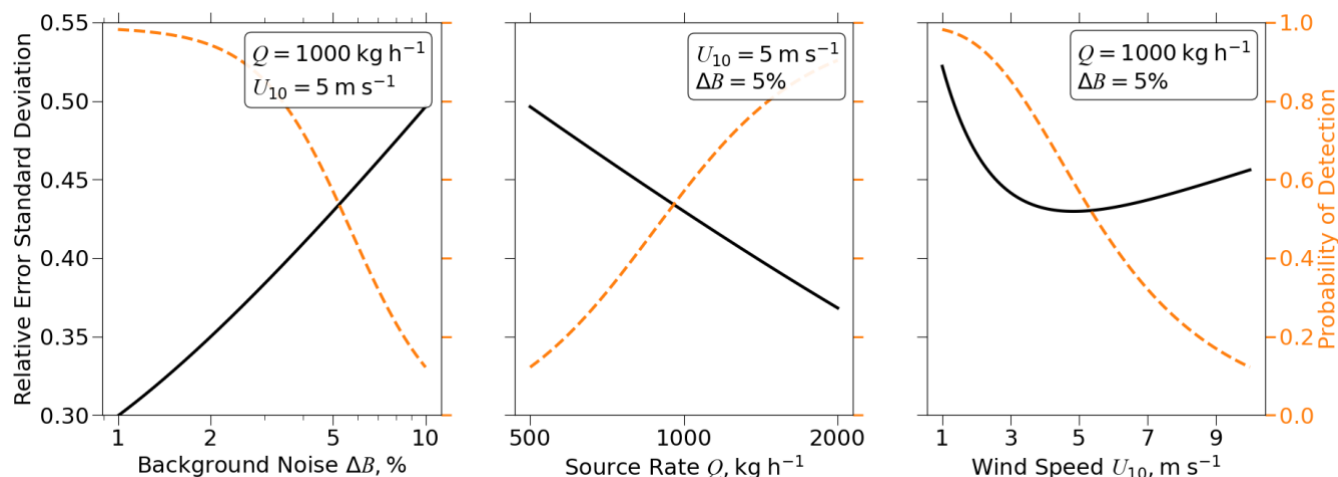
325

Uncertainty in wind speed adds another source of error. Let σ_U (m s^{-1}) denote the error standard deviation in the 10-m wind speed U_{10} . Replacing in equations (2) and (3) yields a corresponding relative error standard deviation $\sigma_{Q,U}$ on the inferred IME source rate Q :

330
$$\sigma_{Q,U} = \frac{0.23 \sigma_U}{0.7 + 0.23 U_{10}} \tag{8}$$

Wind speed data may be available locally or from meteorological analysis datasets. A global default is the NASA Goddard Earth Observation System – Fast Processing (GEOS-FP) data publicly available on a $0.25^\circ \times 0.3125^\circ$ grid at 1-h temporal resolution. Varon et al. (2018) estimated an error standard deviation $\sigma_U = 2 \text{ m s}^{-1}$ for the GEOS-FP data, independent of wind speed magnitude, by comparison to 5-minute observations at US airports. Replacing into equation (8) indicates a maximum relative error standard deviation of 66% at low wind speed, decreasing with increasing wind speed. At high wind speeds the error becomes small but the IME is then small so that the masking error is large as inferred from the inverse dependence of the point source observability on wind speed (equation (4) and Figure 7).

335



340



Figure 8: Total relative error standard deviation σ_Q on point source rate estimates from the U-Plume algorithm with the IME method (equation (9)) as a function of three variables: background noise ΔB (%), source rate Q (kg h^{-1}), and 10-m wind speed U_{10} (m s^{-1}). The dashed orange line represents the probability of point source detection calculated with equation (6).

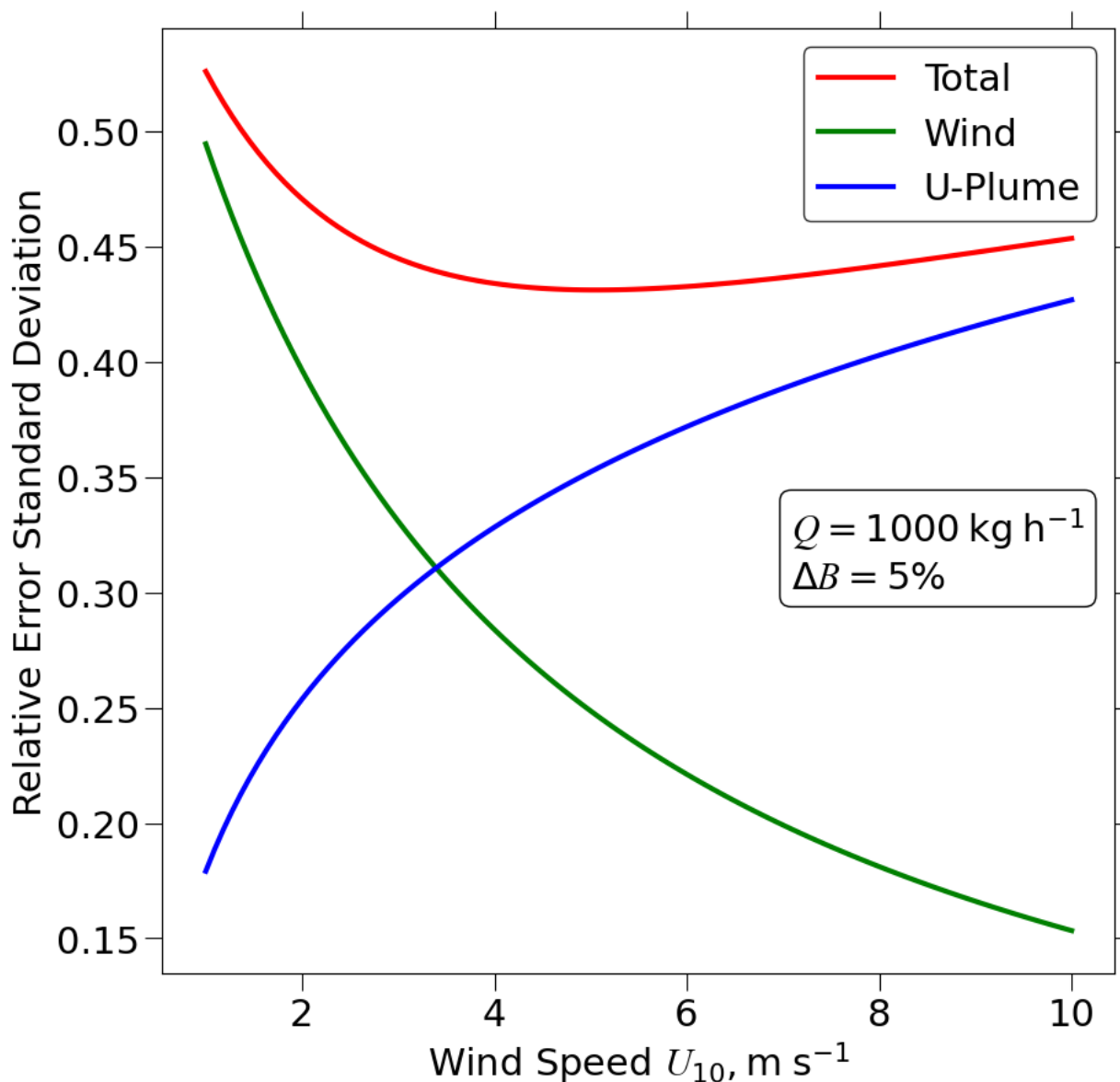
345

Adding the error variances from equations (7) and (8) in quadrature gives the total relative error variance σ_Q^2 on the estimated sources rates from the U-Plume algorithm including error on wind speed:

$$\sigma_Q^2 = (\max(0.1, (0.52 - 0.12 \log(O_{ps})))^2 + \left(\frac{0.23 \sigma_U}{0.7 + 0.23 U_{10}}\right)^2 \quad (O_{ps} > 2) \quad (9)$$

350

Fig. 8 shows the total relative error standard deviation σ_Q as a function of background noise ΔB , source rate Q , and 10-m wind speed, U_{10} . The total relative error standard deviation increases linearly with $\log(\Delta B)$, decreases linearly with $\log(Q)$, and is minimum for $U_{10} = 4 \text{ m s}^{-1}$.



355 M

360

Figure 9: Dependence of errors in point source estimates on wind speed. The Figure shows the relative error standard deviation on the source rate estimates inferred from U-Plume with the IME method (equation (9)) as a function of 10-m wind speed (U_{10}). The total relative error standard deviation σ_Q is shown as the red line (same as Figure 8) and is decomposed into the contributions from errors in the U-Plume algorithm ($\sigma_{Q,M}$ equation (7)) and errors in wind speed (σ_U equation (8)).

The dependence of the total relative error standard deviation on wind speed is partitioned further in Figure 9 into the contributions from the U-Plume algorithm and wind speed errors. The error contribution from the U-Plume algorithm increases



with rising wind speed, because methane enhancements in the plume become smaller, but this levels off at high wind speeds
365 as the plumes are increasingly likely to be undetected instead. The error contribution from wind speed decreases with rising
wind speed. The total error is dominated by wind speed for $U_{10} < 4 \text{ m s}^{-1}$ and by the U-Plume algorithm for $U_{10} > 4 \text{ m s}^{-1}$. For
the range of values of ΔB and Q in our dataset we find that the cross-over between the two regimes is at $2\text{-}4 \text{ m s}^{-1}$, which can
be regarded as an optimum wind speed range for plume quantification.

5 Conclusions

370 We developed the U-Plume algorithm for automated detection and quantification of point source rates from high-resolution
satellite imagery of atmospheric column concentrations. Our work was motivated by the need for fast identification of plumes
in the operational processing of the vast amounts of methane data from the rapidly expanding constellation of GHGSat and
other satellite instruments targeting methane point sources. The method can also be applied to any chemically inert plume such
as for CO_2 .

375

U-Plume involves two steps. The first step is a machine learning U-Net architecture for plume detection and delineation
(masking) in noisy satellite images. The resulting plume mask is then used together with wind speed information in a second
step of source rate quantification using either a convolutional neural network (CNN) or a physically based Integrated Mass
Enhancement (IME) method. Having plume mask as well as source rate information available from U-Plume output is
380 important for visualization, quality control, and pinpointing the source location. The end-to-end algorithm can process 62
images per second on a single core.

We trained U-Plume with an ensemble of plume free observation images from the GHG-Sat C1 satellite instrument covering
a range of surfaces from homogeneous to highly heterogeneous and superimposing instantaneous methane plumes from large-
385 eddy simulations with known point source rates. Evaluation with an independent dataset shows that successful plume detection
and masking is strongly dependent on four state variables: instrument background noise ΔB , source rate Q , 10-m wind speed
 U_{10} , and pixel resolution W . We combine these variables into a new dimensionless number metric, the point source
observability $O_{ps} = Q/(WU_{10}\Delta B)$, and show that this metric can successfully predict the ability of a given plume imaging
instrument to detect the plumes and quantify source rates for given observing conditions. It can assist in determining when
390 automation is possible for a given target detection level. For the GHGSat-C2 instruments with background noise $\Delta B < 1\%$, we
find that U-Plume can reliably detect and quantify point sources with $Q > 400 \text{ kg h}^{-1}$. U-Plume's value comes in the ability to
process large sets of plume data rather than pushing the limits of detectability. Human operators with knowledge of point
source location would be expected to have greater ability to detect small sources (Sherwin et al., 2022).

395 We find that the physically based IME method is superior to the CNN method for inferring point source rates from the plume
masks. The CNN has high bias for low source rates, and low bias for high source rates, as is typical for machine learning



400 methods. The superiority of the IME method would be expected considering that there is a simple physically-based linear relationship between plume mass and source rate modulated by wind speed. Although a CNN method may not require information on wind speed, such information is always available either from local measurements or from regional/global databases.

405 We developed an end-to-end error model for the point source rates inferred from U-Plume as a function of O_{ps} . We find that at low wind speeds the error is dominated by wind speed whereas at higher wind speeds the error is dominated by the U-Plume algorithm. The U_{10} value where this shift occurs is typically 2-4 m s⁻¹. This also represents an optimal wind speed range for plume detection and quantification.

410 U-Plume thus offers a capable tool for fast automated processing of vast amounts of satellite imagery to detect plumes from point sources and quantify point source rates. As the ability of satellite observations to decrease background noise continues to improve, the U-Plume capability to detect and quantify points sources will correspondingly increase.

Acknowledgments. DJJ acknowledges funding from the NASA Carbon Monitoring System.

Data Availability

415 The model weights and both the original training data and the augmented test dataset are available through Harvard Dataverse (<https://doi.org/10.7910/DVN/YFRQU4>).

References

420 Beirle, S., Borger, C., Dörner, S., Eskes, H. J., Kumar, V., De Laat, A., and Wagner, T.: Catalog of NO_x emissions from point sources as derived from the divergence of the NO₂ flux for TROPOMI, Earth Syst. Sci. Data, 13, 2995–3012, <https://doi.org/10.5194/essd-13-2995-2021>, 2021.

425 Bovensmann, H., Buchwitz, M., Burrows, J. P., Reuter, M., Krings, T., Gerilowski, K., Schneising, O., Heymann, J., Tretner, A., and Erzinger, J.: A remote sensing technique for global monitoring of power plant CO₂ emissions from space and related applications, Atmospheric Measurement Techniques, 3, 781–811, <https://doi.org/10.5194/amt-3-781-2010>, 2010.

Buchwitz, M., Schneising, O., Reuter, M., Heymann, J., Krautwurst, S., Bovensmann, H., Burrows, J. P., Boesch, H., Parker, R. J., Somkuti, P., Detmers, R. G., Hasekamp, O. P., Aben, I., Butz, A., Frankenberg, C., and Turner, A. J.: Satellite-derived



methane hotspot emission estimates using a fast data-driven method, *Atmospheric Chemistry and Physics*, 17, 5751–5774, <https://doi.org/10.5194/acp-17-5751-2017>, 2017.

430

Clarisse, L., Van Damme, M., Clerbaux, C., and Coheur, P.-F.: Tracking down global NH₃ point sources with wind-adjusted superresolution, *Atmospheric Measurement Techniques*, 12, 5457–5473, <https://doi.org/10.5194/amt-12-5457-2019>, 2019.

Cusworth, D. H., Jacob, D. J., Varon, D. J., Chan Miller, C., Liu, X., Chance, K., Thorpe, A. K., Duren, R. M., Miller, C. E.,
435 Thompson, D. R., Frankenberg, C., Guanter, L., and Randles, C. A.: Potential of next-generation imaging spectrometers to detect and quantify methane point sources from space, *Atmospheric Measurement Techniques Discussions*, 1–29, <https://doi.org/10.5194/amt-2019-202>, 2019.

Cusworth, D. H., Duren, R. M., Thorpe, A. K., Olson-Duvall, W., Heckler, J., Chapman, J. W., Eastwood, M. L., Helmlinger,
440 M. C., Green, R. O., Asner, G. P., Dennison, P. E., and Miller, C. E.: Intermittency of Large Methane Emitters in the Permian Basin, *Environ. Sci. Technol. Lett.*, 8, 567–573, <https://doi.org/10.1021/acs.estlett.1c00173>, 2021.

Dammers, E., McLinden, C. A., Griffin, D., Shephard, M. W., Van Der Graaf, S., Lutsch, E., Schaap, M., Gainairu-Matz, Y.,
Fioletov, V., Van Damme, M., Whitburn, S., Clarisse, L., Cady-Pereira, K., Clerbaux, C., Coheur, P. F., and Erisman, J. W.:
445 NH₃ emissions from large point sources derived from CrIS and IASI satellite observations, *Atmospheric Chemistry and Physics*, 19, 12261–12293, <https://doi.org/10.5194/acp-19-12261-2019>, 2019.

Duren, R. M., Thorpe, A. K., Foster, K. T., Rafiq, T., Hopkins, F. M., Yadav, V., Bue, B. D., Thompson, D. R., Conley, S.,
Colombi, N. K., Frankenberg, C., McCubbin, I. B., Eastwood, M. L., Falk, M., Herner, J. D., Croes, B. E., Green, R. O., and
450 Miller, C. E.: California’s methane super-emitters, *Nature*, 575, 180–184, <https://doi.org/10.1038/s41586-019-1720-3>, 2019.
Fioletov, V. E., McLinden, C. A., Krotkov, N., and Li, C.: Lifetimes and emissions of SO₂ from point sources estimated from OMI, *Geophysical Research Letters*, 42, 1969–1976, <https://doi.org/10.1002/2015GL063148>, 2015.

de Foy, B., Lu, Z., Streets, D. G., Lamsal, L. N., and Duncan, B. N.: Estimates of power plant NO_x emissions and lifetimes
455 from OMI NO₂ satellite retrievals, *Atmospheric Environment*, 116, 1–11, <https://doi.org/10.1016/j.atmosenv.2015.05.056>, 2015.

Frankenberg, C., Thorpe, A. K., Thompson, D. R., Hulley, G., Kort, E. A., Vance, N., Borchardt, J., Krings, T., Gerilowski,
K., Sweeney, C., Conley, S., Bue, B. D., Aubrey, A. D., Hook, S., and Green, R. O.: Airborne methane remote measurements
460 reveal heavy-tail flux distribution in Four Corners region, *PNAS*, 113, 9734–9739, <https://doi.org/10.1073/pnas.1605617113>, 2016.



465 Guanter, L., Irakulis-Loitxate, I., Gorroño, J., Sánchez-García, E., Cusworth, D. H., Varon, D. J., Cogliati, S., and Colombo, R.: Mapping methane point emissions with the PRISMA spaceborne imaging spectrometer, *Remote Sensing of Environment*, 265, 112671, <https://doi.org/10.1016/j.rse.2021.112671>, 2021.

470 Jacob, D. J., Turner, A. J., Maasackers, J. D., Sheng, J., Sun, K., Liu, X., Chance, K., Aben, I., McKeever, J., and Frankenberg, C.: Satellite observations of atmospheric methane and their value for quantifying methane emissions, *Atmospheric Chemistry and Physics*, 16, 14371–14396, <https://doi.org/10.5194/acp-16-14371-2016>, 2016.

Jervis, D., McKeever, J., Durak, B. O. A., Sloan, J. J., Gains, D., Varon, D. J., Ramier, A., Strupler, M., and Tarrant, E.: The GHGSat-D imaging spectrometer, *Atmos. Meas. Tech.*, 14, 2127–2140, <https://doi.org/10.5194/amt-14-2127-2021>, 2021.

475 Jongaramrungruang, S., Frankenberg, C., Matheou, G., Thorpe, A. K., Thompson, D. R., Kuai, L., and Duren, R. M.: Towards accurate methane point-source quantification from high-resolution 2-D plume imagery, *Atmospheric Measurement Techniques*, 12, 6667–6681, <https://doi.org/10.5194/amt-12-6667-2019>, 2019.

Jongaramrungruang, S., Thorpe, A. K., Matheou, G., and Frankenberg, C.: MethaNet – An AI-driven approach to quantifying methane point-source emission from high-resolution 2-D plume imagery, *Remote Sensing of Environment*, 269, 112809, <https://doi.org/10.1016/j.rse.2021.112809>, 2022.

485 Joyce, P., Ruiz Villena, C., Huang, Y., Webb, A., Gloor, M., Wagner, F. H., Chipperfield, M. P., Barrio Guilló, R., Wilson, C., and Boesch, H.: Using a deep neural network to detect methane point sources and quantify emissions from PRISMA hyperspectral satellite images, *Atmospheric Measurement Techniques*, 2023.

490 Krings, T., Gerilowski, K., Buchwitz, M., Reuter, M., Tretner, A., Erzinger, J., Heinze, D., Pflüger, U., Burrows, J. P., and Bovensmann, H.: MAMAP – a new spectrometer system for column-averaged methane and carbon dioxide observations from aircraft: retrieval algorithm and first inversions for point source emission rates, *Atmospheric Measurement Techniques*, 4, 1735–1758, <https://doi.org/10.5194/amt-4-1735-2011>, 2011.

Krings, T., Gerilowski, K., Buchwitz, M., Hartmann, J., Sachs, T., Erzinger, J., Burrows, J. P., and Bovensmann, H.: Quantification of methane emission rates from coal mine ventilation shafts using airborne remote sensing data, *Atmospheric Measurement Techniques*, 6, 151–166, <https://doi.org/10.5194/amt-6-151-2013>, 2013.



- 495 Maasackers, J. D., Varon, D. J., Elfarsdóttir, A., McKeever, J., Jervis, D., Mahapatra, G., Pandey, S., Lorente, A., Borsdorff, T., Foorhuis, L. R., Schuit, B. J., Tol, P., van Kempen, T. A., van Hees, R., and Aben, I.: Using satellites to uncover large methane emissions from landfills, *Science Advances*, 8, eabn9683, <https://doi.org/10.1126/sciadv.abn9683>, 2022.
- McLinden, C. A., Fioletov, V., Krotkov, N. A., Li, C., Boersma, K. F., and Adams, C.: A Decade of Change in NO₂ and SO₂ over the Canadian Oil Sands as Seen from Space, *Environ. Sci. Technol.*, 50, 331–337, <https://doi.org/10.1021/acs.est.5b04985>, 2016.
- 500 Nassar, R., Hill, T. G., McLinden, C. A., Wunch, D., Jones, D. B. A., and Crisp, D.: Quantifying CO₂ Emissions From Individual Power Plants From Space, *Geophysical Research Letters*, 44, 10,045–10,053, <https://doi.org/10.1002/2017GL074702>, 2017.
- 505 Noppen, L., Clarisse, L., Tack, F., Ruhtz, T., Merlaud, A., Van Damme, M., Van Roozendaal, M., Schuettemeyer, D., and Coheur, P.: Constraining industrial ammonia emissions using hyperspectral infrared imaging, *Remote Sensing of Environment*, 291, 113559, <https://doi.org/10.1016/j.rse.2023.113559>, 2023.
- 510 Pommier, M., McLinden, C. A., and Deeter, M.: Relative changes in CO emissions over megacities based on observations from space, *Geophysical Research Letters*, 40, 3766–3771, <https://doi.org/10.1002/grl.50704>, 2013.
- Ramier, A., Girard, M., Jervis, M., MacLean, J.P., Marshall, D., McKeever J., Strupler, M., Tarrant, E., and Young, D.: High-Resolution Methane Detection with the GHGSat Constellation, in: GLOC 2023 conference proceedings, 75002, 2023.
- 515 Rezvanbehbahani, S., Stearns, L. A., Keramati, R., Shankar, S., and van der Veen, C. J.: Significant contribution of small icebergs to the freshwater budget in Greenland fjords, *Communications Earth & Environment*, 1, 1–7, <https://doi.org/10.1038/s43247-020-00032-3>, 2020.
- 520 Ronneberger, O., Fischer, P., and Brox, T.: U-Net: Convolutional Networks for Biomedical Image Segmentation, *arXiv:1505.04597 [cs]*, 2015.
- Valin, L. C., Russell, A. R., and Cohen, R. C.: Variations of OH radical in an urban plume inferred from NO₂ column measurements, *Geophysical Research Letters*, 40, 1856–1860, <https://doi.org/10.1002/grl.50267>, 2013.
- 525 Varon, D. J., Jacob, D. J., McKeever, J., Jervis, D., Durak, B. O. A., Xia, Y., and Huang, Y.: Quantifying methane point sources from fine-scale satellite observations of atmospheric methane plumes, *Atmospheric Measurement Techniques*, 11, 5673–5686, <https://doi.org/10.5194/amt-11-5673-2018>, 2018.

<https://doi.org/10.5194/egusphere-2023-1343>

Preprint. Discussion started: 25 August 2023

© Author(s) 2023. CC BY 4.0 License.



Varon, D. J., Jacob, D. J., Jervis, D., and McKeever, J.: Quantifying Time-Averaged Methane Emissions from Individual Coal
530 Mine Vents with GHGSat-D Satellite Observations, Environ. Sci. Technol., 54, 10246–10253,
<https://doi.org/10.1021/acs.est.0c01213>, 2020.