Performance and sensitivity of column-wise and pixel-wise methane retrievals for imaging spectrometers

Alana Ayasse[1,2], Daniel Cusworth[1,2], Kelly O'Neill[1], Andrew Thorpe[3], and Riley Duren[1,2,3]
[1]Carbon Mapper
[2]University of Arizona
[3]Jet Propulsion Laboratory

Corresponding author: Alana Ayasse, alanaayasse@arizona.edu

Introduction

Airborne imaging spectrometers, like the Global Airborne Observatory (GAO) measure solar backscattered radiance. GAO in particular measures solar backscatter between 400-2500 nm at 5 nm spectral resolution. This allows for retrieval of methane (CH4) concentrations at high spatial resolution (e.g., 3-5 m when aircraft flies between 3-5 km). CH4 retrieval algorithms take many forms, but two common algorithm approaches are (1) the columnwise matched filter (CMF), and (2) the physics-based Iterative Maximum A Posteriori – Differential Optical Absorption Spectroscopy (IMAP-DOAS). CMF algorithms are computationally fast and use scene or column-level statistical properties to retrieve CH4 concentrations. IMAP-DOAS is slower computationally but each pixel's CH4 concentration is retrieved independently. Due to computational tractability and good agreement with previous controlled release experiments (e.g., Duren et al., 2019; Thorpe et al., 2017; Thorpe et al., 2016), CMF approaches have been applied frequently for basin-scale CH4 mapping.

The single-blind controlled release (CR) experiment undertaken by Stanford in Summer 2021 was an additional opportunity to test algorithm performance (Rutherford et al., in prep). To optimize multiple overpasses of the CR site over the 3 day duration of the campaign, very short flight lines were flown by GAO of average 3km in length (1200 pixels in along-track pixels), resulting in 200 overpasses of the CR site. These lines were atypically smaller than standard campaign operations by Carbon Mapper (Figure 1). In what follows, we show how these short flight lines introduced a statistical bias into the CMF algorithm, which propagated into emission calculations. We provide additional evidence of this CMF bias by performing IMAP-DOAS comparisons at the CR site. We also artificially truncate previously flown Permian flight lines, running the CMF retrieval and comparing to standard operations. The results from these analyses point clearly to the fact that these unrepresentative short flight lines cause underestimation in CMF-based emission estimates.

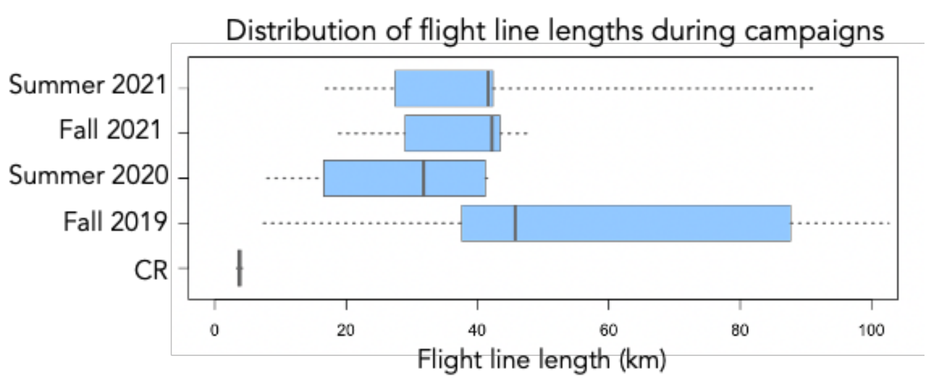

Figure 1. Flight line lengths during the summer 2021 controlled release (CR) experiment compared to Carbon Mapper Permian field campaigns (Cusworth et al., 2021; Cusworth et al., 2022).

Methods

<u>Columnwise Matched Filter (CMF)</u>

Carbon Mapper's standard operating pipeline employs a CMF algorithm, which takes the following form (Thomspon et al., 2016):

$$\hat{\alpha}(\mathbf{x}) = (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} \mathbf{t} \,/ (\mathbf{t}^T \boldsymbol{\Sigma}^{-1} \mathbf{t})$$

Where $\hat{\alpha}$ is the concentration enhancement, $\mathbf{x}$ is a radiance spectrum, $\boldsymbol{\mu}$ is the mean radiance spectrum in an along-track column, $\boldsymbol{\Sigma}$ is a covariance matrix, and $\mathbf{t}$ is a unit absorption spectrum. In essence, the matched filter uses statistics from all pixels in a flight column to assess whether a single pixel's spectrum is enhanced by methane (i.e., has deeper absorption features). This requires sufficient column-wise statistics. Some statistical intuition and rules of thumb suggested that the dimension of a column should be at least seven times larger than the covariance matrix dimension, and that no columns should have more than 5% of its pixels enhanced by methane. During the controlled release experiment, Carbon Mapper attempted to maximize the number revisits given during the relatively short duration of the test. This led to very short flight lines (average 1200 pixels per column), which put us near the statistical limit for the matched filter according to these rules of thumb.

Iterative Maximum A Posteriori – Differential Optical Absorption Spectroscopy (IMAP-DOAS)

IMAP-DOAS estimates column-average methane concentrations on a per-pixel basis by simulation of top of the atmosphere radiance and inversion (or retrieval) for the best atmospheric parameters that reduce mismatch between an observed spectrum and a simulated spectrum, assuming some prior constraints. For a simulation spectrum, IMAP-DOAS uses a radiative transfer model that relies on a multi-layered Beer-Lambert Law equation to simulate high frequency atmospheric features and a multi-dimensional polynomial to represent low-frequency reflectance and scattering features (Cusworth et al., 2019):

$$F^{\mathrm{h}}(\boldsymbol{x}) = I_0(\lambda)\exp\left(-A\sum_{n=1}^{3} s_n \sum_{l=1}^{72} \tau_{n,l}\right)\sum_{k=0}^{K} a_k P_k(\lambda).$$

Where $\boldsymbol{I}_0$ is the solar spectrum, A is the geometric airmass factor, s and τ are scaling factors or optical depths for either CH4, H2O, or N2O, and a is a polynomial coefficient. IMAP-DOAS has been used in multiple previous studies for a smaller population of emission sources (Cusworth et al., 2020; Cusworth et al., 2019; Thorpe et al., 2017; Thorpe et al., 2014) but is currently not run operationally for our larger area surveys due to computational constraints. Generally, a single-pixel retrieval takes a few seconds. In airborne surveys, we routinely capture imagery that have 600 × 5000+ pixels. Simulation of an entire flight line if done sequentially, in this case, would take 35 days to complete. The CMF, by contrast takes less than 1 minute to process the entire flight line. Because of these computational limits, IMAP-DOAS for this study has not been tuned for every heterogeneous surface condition. In practice, this retrieval is therefore generally applied for research applications on a small number of plumes, where retrieval parameters can be optimized for particular scene conditions. For some time, Carbon Mapper has been evaluating the possibility of using plume detection with the CMF algorithm to trigger follow-up emissions quantification using IMAP-DOAS but this functionality is not yet implemented in our operational analysis system for the aircraft.

The benefit of IMAP-DOAS is that (1) each retrieved pixel is independent and (2) that retrieval uncertainties can be explicitly characterized by the Bayesian formulation of the retrieval. This contrasts with the CMF approach, where the retrieved concentration for a single pixel depends on the quality and density of pixels in an acquisition (e.g., a single along-track column).

For both CMF and IMAP-DOAS, we estimate emission rates via the Integrated Methane Enhancement (IME) method (Frankenberg et al., 2016; Duren et al., 2019). For winds speeds, we used U10 fields from the HRRR reanalysis.

Results

Estimated airborne emission rates compared to metered emissions (e.g., the "ground truth") are shown in Figure 2 for both CMF and IMAP-DOAS. An ordinary least squares (OLS) fit between the CMF results and the metered emissions results in $y = 0.31x + 98$ with $R^2 = 0.34$. An OLS fit between IMAP-DOAS and metered emissions results in $y = 1.04x - 26$ with $R^2 = 0.71$. The CMF approach therefore is significantly underestimating metered emission rates, and showing poor correlation. This problem in bias and accuracy largely is mitigated when applying a physics-based retrieval.

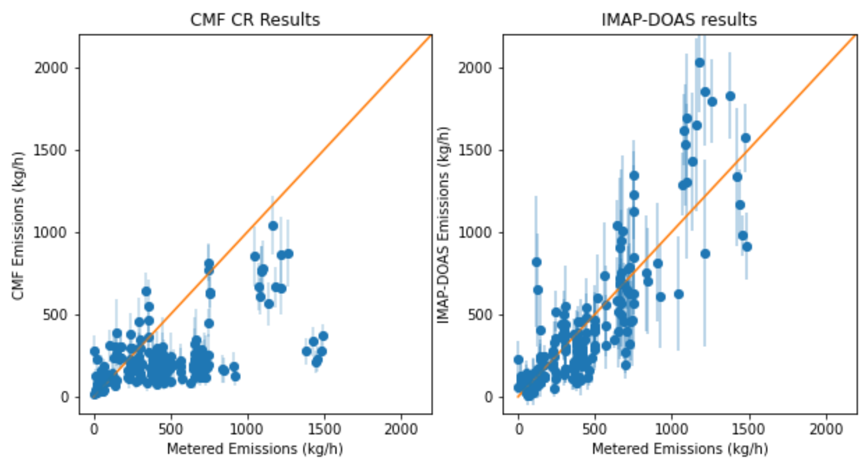

Figure 2. CMF and IMAP-DOAS comparison to metered emission rates. An OLS fit to CMF results in $y = 0.31x + 98$ *with* $R^2 = 0.34$*. An OLS fit to IMAP-DOAS results in* $y = 1.04x - 26$ *with* $R^2 = 0.71$*.*

IMAP-DOAS does not rely on long flight lines for quantification, so the much closer agreement to metered emission rates in Figure 2 is strong evidence that short flight lines drove much of the bias during the CR experiment. To provide further evidence for this point, we selected a subset of 50 flight lines that were flown during standard campaign operations in the Permian between 2019-2021. We isolated a single unique plume in each line, cropped the scene around that plume such that it was 1200 pixels in the along-track direction, and then ran the CMF algorithm. These cropped scenes are representative of the statistical sampling conditions also present in the CR CMF results.

Figure 3 shows the results of cropping 2019-2021 Permian scenes to the same pixel dimension as the CR experiment. What is immediately obvious is that estimated emissions from these cropped scenes are much lower than the standard CMF emission estimates that use all pixels in the along-track direction. An OLS fit between the cropped and standard CMF emissions results in $y = 0.14x + 81$ with $R^2 = 0.47$, showing a severe reduction in estimated emissions. Since there is uncertainty in Figure 3 in both variables, a reduced major axis (RMA) regression fit may be more appropriate, which results in $y = 0.20x + 19$ (same R^2), on-par with the CMF results in Figure 2. This lends additional evidence that the poor results in Figure 2 were driven primarily by short flight lines.

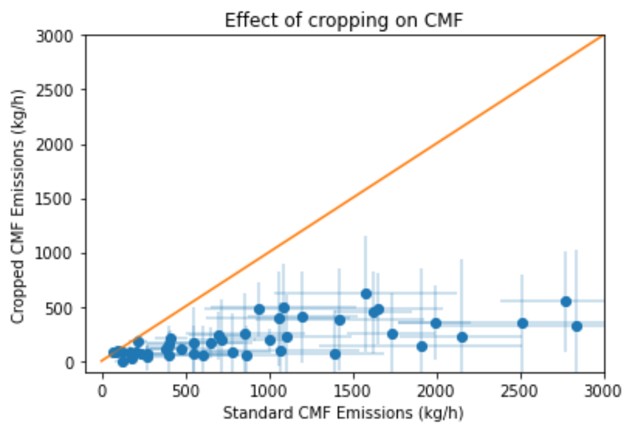

Figure 3. Effect of cropping flight lines on CMF results. Flight lines were taken from 2019-2021 Permian campaigns that were flown under normal operations (Figure 1), then cropped to 1200 pixels, and the CMF was reran. The resulting emissions are compared to the emissions from the standard full-line CMF processing.

Figures 2-3 present strong evidence that short flight lives severely affected CMF performance during the CR experiment. However, there still remains the broader question of in-field quantification performance of Carbon Mapper's operational CMF algorithm under longer, more representative flight lines (e.g., 20-50+ km) and whether any adjustments are warranted. To test the representativeness of the standard CMF-based analysis from field-campaigns, we apply IMAP-DOAS on a representative subset of plumes, estimate emissions, and compare to the standard CMF results. Here, this subset includes 60+ plumes that relate to 20 distinct facilities that were imaged on at least 3 separate days during airborne campaigns by the Global Airborne Observatory during the Fall 2019, Summer 2020, Summer 2021, and Fall 2021 campaigns. These plumes represent a dynamic range of emission rates reported by the CMF algorithm (90 kg/h – 3900 kg/h) that represent a diversity of infrastructure types in this region.

The results of the IMAP-DOAS to CMF comparison are shown in Figure 4. The left panel shows instantaneous plume-to-plume emission comparison for the different retrieval approaches. The data comparison shows general agreement between the two retrieval approaches. An OLS fit results in $y = 0.72x + 307$ with $R^2 = 0.67$. Applying an RMA fit in Figure 4a results in $y = 0.84x + 383$ with the same R^2 value.

In practice, we use persistence-adjusted average emissions when summarizing the results from campaigns and constructing emission budgets for regions or facilities (Cusworth *et al.,* 2021). The right panel of Figure 4 shows the comparison of IMAP-DOAS to CMF after averaging and applying persistence adjustment to the emissions. Here, the comparison between retrieval approaches shows very close correspondence: OLS fit: $y = 0.89x + 120$ with $R^2 = 0.82$; RMA fit: $y = 0.99x + 58$. As expected, the variability in emissions on a plume-by-plume basis gets averaged out in Figure 4b.

We also ran this comparison for 200 individual plume estimates across the 2019, 2020 and 2021 Permian campaigns which resulted in an OLS fit of $y = 0.82x + 233$ with $R^2 = 0.74$ (RMA regression $y = 0.95x + 168$).

We underscore that IMAP-DOAS does not represent a "ground-truth," but given the good agreement of IMAP-DOAS with CR metered emission rates in Figure 2, to have confidence in quantification of the operational CMF data analysis system used in the field campaigns, we would expect CMF results to show good correlation to IMAP-DOAS. This is indeed the case, although with some variability and uncertainty on an individual plume by plume basis.

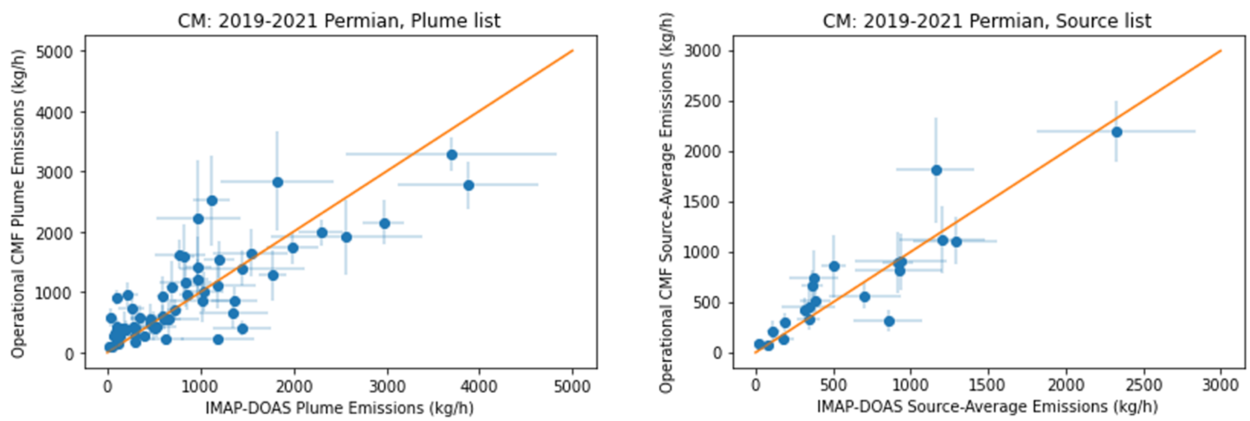

Figure 4. Comparison of emission rates for a subset of 2019-2021 plumes in the Permian Basin between the operational CMF analysis system and IMAP-DOAS. Error bars represent 1-sigma uncertainties on emissions. Regression fits for left panel (plume list with instantaneous emissions): OLS: $y = 0.72x + 307$ *with* $R^2 = 0.67$; $RMA : y = 0.84x + 383$. *Regression fits for the right panel (source list with average emissions): OLS: OLS:* $y = 0.89x + 120$ *with* $R^2 = 0.82$; $RMA : y = 0.99x + 58$

<u>Conclusions</u>

The non-standard short flight lines flown during the 2021 CR experiment resulted in an unexpected low bias in CMF retrieved CH_4 concentrations which propagated into low emission rates. Here, we tested that hypothesis by applying the pixelwise IMAP-DOAS retrieval to the CR experiment. We found a much-improved result, with IMAP-DOAS derived emission rates showing strong correlation and little bias across the experiment. We also artificially crop flight lines from 2019-2021 Permian flights to match the pixel resolution as the CR experiment, reprocess the CMF, and show a reduction in emissions on-par with the CR CMF results.

In order to evaluate the potential for bias in emission estimates from previous Carbon Mapper campaigns that employed the operational CMF algorithm, we performed IMAP-DOAS simulations on a subset of sources detected in the Permian between 2019-2021. We find some scatter, but generally good correlation and low bias between retrieval approaches across this entire population. Attempting to adjust CMF-derived emission rates for the Permian using

IMAP-DOAS would likely result only in a minor change in estimated emissions within the original uncertainties. Given the good correlation/low bias of IMAP-DOAS with CR metered emission rates and the good correlation/low bias of IMAP-DOAS with operational CMF emission rates, we conclude that the CMF results from the 2021 CR experiment are not representative of Carbon Mapper's current operational airborne observing system.

Based on this analysis, we conclude that the previously released CMF-based emission estimates for the Permian basin are in family with uncertainties in prior studies and do not recommend making adjustments based on the 2021 CR experiment. To improve confidence in quantification going forward, we do recommend controlled release experiments that strictly follow standard Carbon Mapper conventions for airborne observations even if it results in fewer samples. As described above, we also plan to further explore the possibility of modifying our operational data analysis system to generate both CMF and IMAP-DOAS emission estimates for improved diagnostics and confidence in uncertainty quantification.

References

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