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DOI

[10.1117/12.3063819](https://doi.org/10.1117/12.3063819)

Publication date

2025

Document Version

Final published version

Published in

Earth Observing Systems XXX

Citation (APA)

Siemons, M., & Kohlhaas, R. (2025). A photonic-crystals enabled spectrometer for remote sensing of greenhouse gases. In X. Xiong, J. S. Czapla-Myers, A. Angal, & J. A. Barsi (Eds.), *Earth Observing Systems XXX* Article 1361103 (Proceedings of SPIE - The International Society for Optical Engineering; Vol. 13611). SPIE. <https://doi.org/10.1117/12.3063819>

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A photonic-crystals enabled spectrometer for remote sensing of greenhouse gases

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ABSTRACT

As global climate change poses one of the most important challenges this century, there is an increasing demand to monitor trace gases with high spatial and temporal resolution. To accomplish this these instruments need to be compact to have constellations of satellites or be able to be equipped on High Altitude Platform Systems. Recently, we introduced a novel highly compact spectrometer instrument concept for trace gas retrieval, making use of photonic crystal filters instead of traditional diffraction based optics. Here the photonic crystal filter transmission profiles are specifically tailored to retrieve the desired trace gases. A particular challenge for this new type of instrument is the design optimization. In addition to traditional performance trade-offs, such as SNR (F-number) and system complexity, the photonic crystal transmission functions also depend on the F-number of the system. Since it is extremely computationally demanding to compute the transmission of many filters for different F-numbers (brute-force optimization approach), a more tailored method is needed. In this work we present a method how to perform a trade-off regarding F-number and trace gas retrieval performance by pre-selecting filters and analyze the performance for these filters as function of F-number. These results show, for the first time, that the sensitivity of the photonic crystal filters to the F-number of the system can substantially degrade the performance compared to only SNR based optimization. It appears that the pre-selected filters, for which the analysis is performed, are particular sensitive the the F-number of the system. This indicates the need for a method to identify robust photonic crystal transmission profiles.

Keywords: Remote Sensing, computational spectroscopy, trace gas retrieval, photonic crystals

1. INTRODUCTION

The need for monitoring greenhouse gas emission sources motivates the development of earth observation systems with higher spatial and temporal resolution. For this complete distributed systems with many satellites could be considered, which would require small, low-weight optical imaging spectrometers. Alternatively, small low-weight spectrometers could be mounted on High Altitude Platform Systems (HAPS) which typically cruise with a speed around 100 km/h at a high around 20 km (60.000 ft).

Conventional grating spectrometers need a large free-space optical path length for the separation of wavelengths and have therefore intrinsic physical limits on the size of the system. Other solutions, for example static Fourier-transform spectrometers as developed with NanoCarb,¹ suffer less from such limitations but have reduced spectral resolution. Recently, a spectrometer concept was invented^{2,3} which uses an array of photonic crystal filters with quasi-random spectral transmission functions. Together with computational inversion (for example compressive sensing) such a system can be use to retrieve trace gas concentrations. Based on this concept we have introduced a novel instrument concept, using compressive sensing enabled by photonic crystals, see Figure 1 and have described this instrument in previous work.⁴ In short, the instrument orbits or flies over the earth and consists of an earth observing optical telescope, where photonic crystals are positioned on the sensor. These photonic crystals consist of a wafer with a thin dielectric material. In our case this is a glass wafer with a 900 nm thin amorphous Si-film with an additional 3 um layer of SiO₂ on top. The aSi-layer contains 2D photonic

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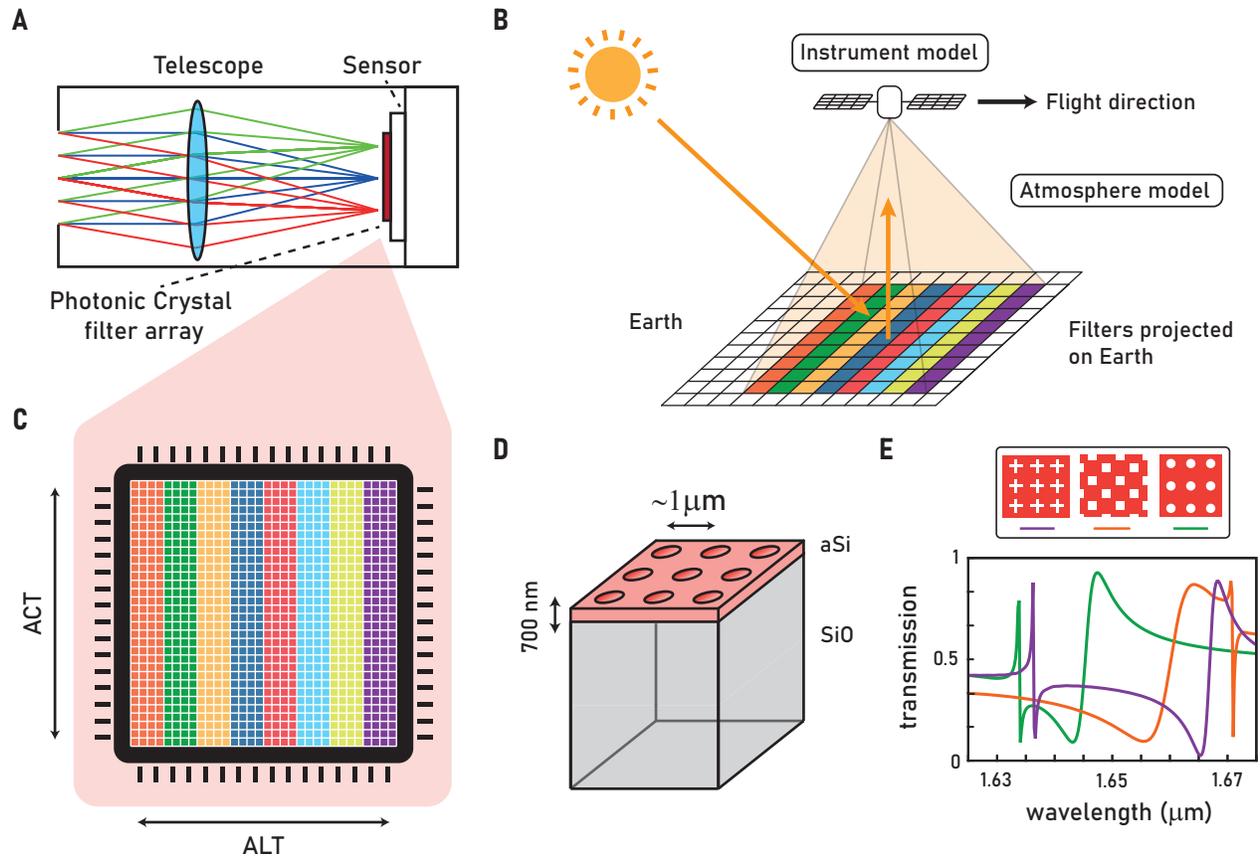


Figure 1. Illustration of the instrument concept. A) The instrument consists of a telescope and sensor. A photonic crystal filter array is placed directly on the sensor. B) As the instrument flies over the earth, ground pixels are observed with different filters. C) The photonic crystals filter array consists of strips in the across track direction. D) The photonic crystal filters itself is made with a small layer of amorphous silicon (aSi) on top of a quartz substrate. In the aSi-layer 2D patterns are etched, giving rise to distinct and spectrally rich transmission profiles (E).

crystals in a column-wise arrangement in the across-track (ACT) direction. These photonic crystals consist of sub-wavelength features etched in the Si-film and have unique spectral transmission profiles. These transmission profiles arise from resonances in the Si-film and depend on the thickness of the film as well as the specific shape and size of the etched structure and the lattice size. By choosing a specific hole shape and lattice size, different spectral transmission profiles can be achieved. The additional SiO₂ layer allows the photonic crystal chip to be bounded to the detector without affecting the transmission profiles. Using the push-broom concept, the transmitted intensity for each ground instantaneous field of view pixel can be measured for each spectral filter. From the measured detector values and the known transmission profiles, the trace gas concentration can be estimated using a retrieval algorithm and atmosphere model.

Such an instrument design allows for a far larger field-of-view in along-track (ALT) direction compared to an imaging spectrometer with a slit and therefore collects more light. This concept has similarities with a linear gradient filter,⁵ but the photonic crystal transmissions allow for a more diverse transmission profiles and a highly tuned and selective optical system. Moreover, different spectral ranges can be combined on one detector (for example the O₂A band and methane band, or several relevant methane spectral ranges).

A particular interesting advantage is that the photonic crystal filters can be chosen to optimize the information measured by the instrument to tailor trace gas retrieval. We have previously described a method how to perform this challenging filter selection based on Fisher Information.⁶ The next challenge in the instrument design is to optimize the F-number (or NA) of the telescope. In traditional instruments, faster optics (low F-number) allow

for a larger etendue and SNR at the cost of optical performance (aberrations) and complexity. The photonic crystal filters add an additional consideration to this trade-off.

The photonic crystal transmission depends on the NA of the focused beam, as the filters are positioned in the focus of the telescope. Therefore, the focused beam transmission profile should be used in the optimization of the instrument design. However, computing the transmission for a focused beam is computationally time consuming. We recently developed a method to efficiently evaluate the transmission for different F-numbers by combining the electric and magnetic fields of different angled plane wave simulations.⁷ In this work we investigate the trade-off in F-number optimization by simulating filters transmission profiles for a range of F-numbers and evaluate the performance.

2. INSTRUMENT MODELING

The instrument and atmosphere model has been described before.⁶ In short, we model the expected intensity for each filter as

$$\mu_k = t_{\text{int}} G N_{\text{pxl}} \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} QE(\lambda) T_k(\lambda) S(\lambda) d\lambda \quad (1)$$

with t_{int} the integration time per image, G the etendue of the instrument, QE the quantum efficiency of the detector, T_k the filter transmission function of the photonic crystal in front of pixel k , N_{pxl} the number of pixels with filter k and S the spectral radiance of the earth. Assuming nadir observation, the etendue G is computed as

$$G = \frac{A \times \text{giFOV}^2}{h^2} \quad (2)$$

with A the aperture size in m^2 , giFOV the ground-instantaneous field of view and of the earth and h the altitude. This can be a low earth orbit (LEO) or the cruising altitude of the HAPS. As a detector the Lynred Snake InGaAs detector is used in low-gain and integrate-while-read mode. This detector has 512×640 pixels, a full well capacity of $1.4 \cdot 10^6 e^-$, a pixel size of $15 \mu\text{m}$ and we assume a QE of 85%. For the spectral radiance of the earth we use a non-scattering radiative transfer model and assume Lambertian reflection at the surface and a standard atmospheric profile. This model ignores cloud properties and atmospheric scattering. More details can be found here.⁸

The radiance spectrum associated with the standard profile is shown in Figure 2. CO₂ has absorption features between 1590–1620 nm and CH₄ has features at 1630–1670 nm and in particular around 1665 nm.

2.1 Trace gas retrieval and performance evaluation

In this work we investigate the performance of CH₄ and CO₂ retrieval in combination with a linearized albedo. This results in fit parameters θ for the enhancement factors χ of CH₄, CO₂ and H₂O and the linearized earth's albedo with two coefficients A_0 and A_1

$$\theta = \begin{bmatrix} \chi_{\text{CH}_4} \\ \chi_{\text{CO}_2} \\ \chi_{\text{H}_2\text{O}} \\ A_0 \\ A_1 \end{bmatrix} \quad (3)$$

The trace gas concentrations and albedo are estimated using a least-squares fit

$$\min_{\theta} (n_k - \mu_k(\theta))^2 \quad (4)$$

with n_k the measured photon count for filter k and μ_k the expected model photon count and θ the fit parameter vector. The least-square fit is efficiently performed with the function `optimize.least_squares` and 'dogbox' method from the python `scipy` library.

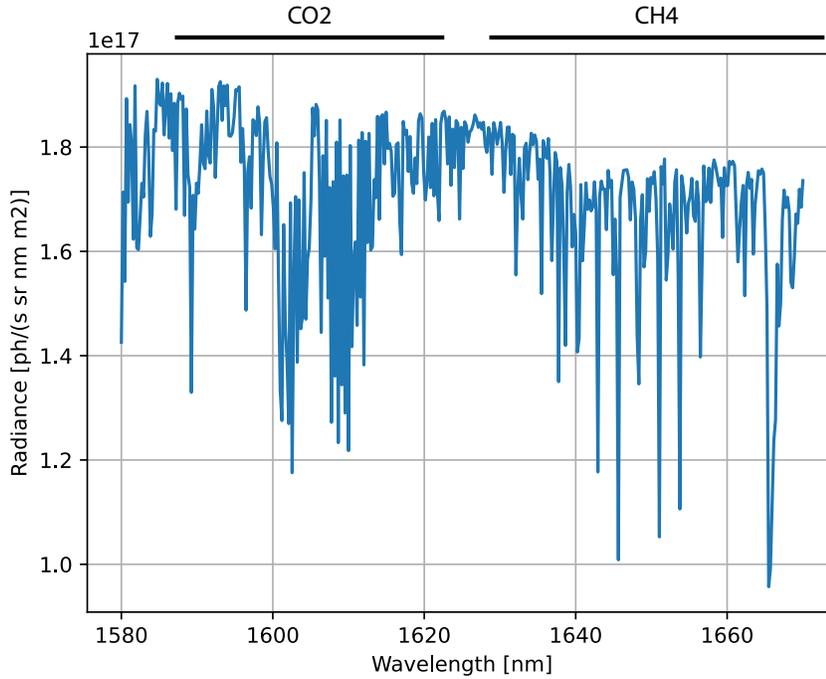


Figure 2. Modeled radiance as function of wavelength. Bars on top indicate the most prominent absorption features of CO2 and CH4.

For the performance of the instrument, both the achieved precision as well as bias (accuracy) of the retrieval are important. A metric which combines both the bias and the precision is the Root Mean Square error (RMSE) of fit parameter i

$$\text{RMSE}_i = \sqrt{\frac{1}{N} \sum_n (\theta_i^n - \theta_i)^2} \quad (5)$$

with θ_i^n the fitted value of noisy realization n , θ_i the ground truth value and N the total amount of noisy realization. Alternatively, the RMS error can be seen as an orthogonal combination of the bias and standard deviation (precision)

$$\text{RMSE}_i = \sqrt{\sigma_i^2 + b_i^2} \quad (6)$$

with $b_i = \bar{\theta}_i - \theta_i$ the bias, $\sigma_i = 1/(N - 1) \sum_n (\theta_i^n - \bar{\theta}_i)^2$ the standard deviation and $\bar{\theta}_i$ the sample mean.

2.2 Instrument configurations

The performance is evaluated for two different configurations: an instrument on a satellite platform in Low Earth Orbit (LEO) with a 10 km FoV and an instrument onboard a High Altitude Platform System (HAPS) with a 1 km FoV. See Table 1.

3. FILTER SIMULATIONS AND SELECTION

The transmission of the filters are simulating using Finite Difference Time Domain (FDTD) using Lumerical. For an initial run a library of 4500 filters transmissions is created with plane wave illumination. From these 4500 filters the best 32 filters are selected, with a selection method described before.⁶ This method is based on optimized the Fisher Information provided by the different filter combinations. Since this computational estimation of the performance of the instrument is (very) quick, trillions of different filter combinations can be tested in a reasonable time. Then for a handful of combinations, the performance can be evaluated through the instrument model.

Table 1. Configuration under study. A Low Earth Orbit configuration and a High Altitude Platform System configuration.

	LEO	HAPS
Altitude (km)	5100	20
Speed over ground (km/h)	6900	100
Spatial Sampling Distance (m)	20 x 20	2 x 2
Ground Resolution Element (m)	50 x 50	2 x 2
Field of View (m)	10.000	1.000
Focal length (m)	0.125	0.15
Forward Motion Compensation	10	-

Next, for a selection of 32 filters the focused beam transmission is computed, based on a method using field synthesis.⁷ This using angular plane wave decomposition to reconstitute the electric magnetic fields of the focused beam for arbitrary F-numbers and is much faster than simulation the complete focused beam for different F-numbers independently. Nonetheless, the computational time required to simulate these 32 filters up to f-number 5 was roughly 1.5 months on a workstation (Intel Xeon Silver 4108, 383 GB RAM). Lastly, we created filter sets using the previously described method selected the best performing sets. We choose filters sets with 16 different filters and computed the performance.

The complete process is therefore as follows:

1. Simulate 4500 filters with plane wave illumination
2. Perform filter selection to identify best 32 filters
3. Compute transmission for focused beams with different F-numbers
4. Perform filter selection with focused beam transmissions for each F-number
5. Evaluate performance for each F-number

For the instrument performance evaluation, the instrument parameters are updated for each different F-number. Faster optics allows for more light collection, which improves SNR. However, the filters transmission profiles smoothen and less information is captured by the filters. Additionally, the larger etendue of small F-numbers requires a faster read-out in order to prevent saturation. This in turn increases the read-out noise as more frames are coadded for a single image. All these components are included in the instrument model.

4. RESULTS AND DISCUSSION

Figure 3 shows a selection of transmission profiles for the 32 selected filters for plane-wave illumination. It is clear that the transmission profiles contain features matching the absorption features of methane and CO₂, as seen in earlier work.⁶ Figure 3 shows the transmission profile for a selected filter for different F-numbers. It appears that for this particular filter, the transmission is quite sensitive to the F-number. The initial reflection feature at 1640 nm completely vanishes for f/6 and even becomes a transmission feature for f/5. Furthermore, the transmission profile for the focused beam is less smooth around 1660 nm due to the computational limitations of the simulation. To achieve reasonable computational time the precision of the simulation has been reduced, leading to small remainders of so called ringing artifacts. It is expected that the features will smooth out with increased simulation precision. Next we evaluated the performance for the two instrument configuration as function of F-number as shown in Figure 4. These results show that faster optics improve the performance of the instrument, albeit not as much as expected just by SNR. This is attributed to the changes in the transmission filters. The best performance achieved by both instruments is Xx and XX. There is a substantial degradation in performance for the focused beam transmission filters compared to the plane-wave transmission profiles. It appears that the 32 selected filters are relatively affected by the focused beam difference compared to other filters.⁷ Therefore, an improved method is needed to select filters which are robust against focused beam illumination, based on the type of resonances inside the photonic crystals.

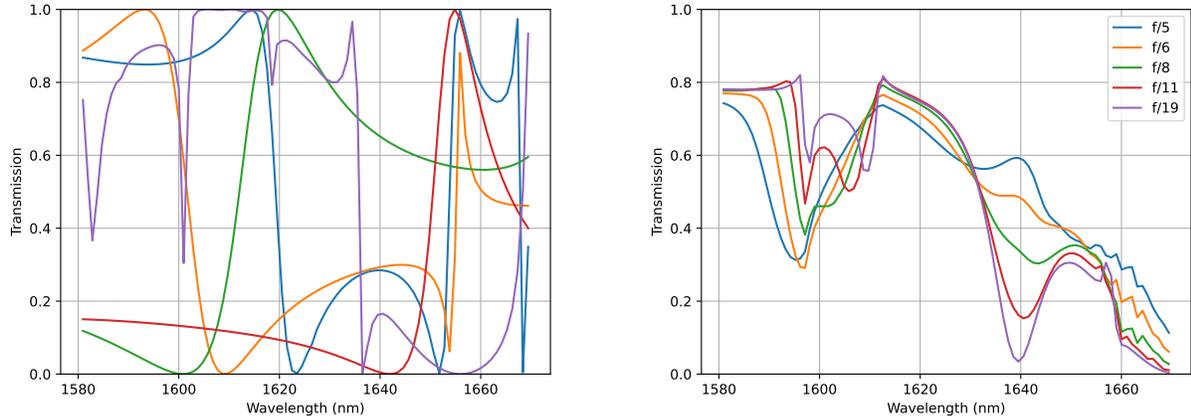


Figure 3. Left: example transmission profiles for plane-wave illumination. Right: transmission profile as function of F-number for an example photonic crystal filter.

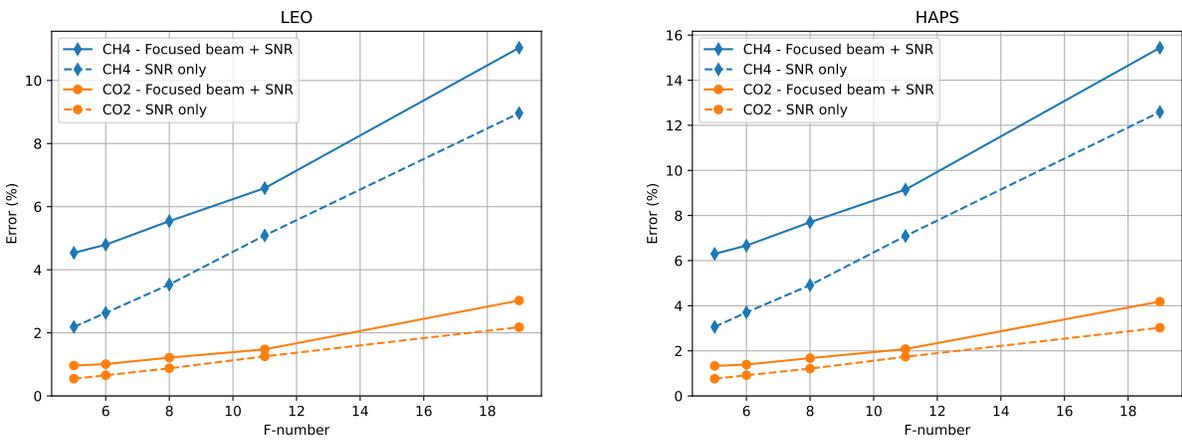


Figure 4. Performance for the 2 instrument configurations (Left: LEO. Right: HAPS) as function of F-number with the correct focused beam transmission or only SNR improvement.

5. CONCLUSION

Here we show a first iteration for a method to optimize photonic crystal enabled spectrometers for remote sensing of greenhouse gases. This method uses a pre-selection to select 32 filters, for which the focused beam transmission are computed, decreasing the computational time to achievable quantities. The predicted performance improves with faster optics, but not as much as can be expected based on SNR only. This is due the smoothing of the filter transmission, decreasing the information captured by each filter as function of F-number. Furthermore, the performance appears to be substantially degraded by the focused beam, indicating that the 32 selected filters are particular sensitive to the focused beam. This highlights the need to incorporate this sensitivity into the filter pre-selection. In conclusion, this work shows that a holistic approach should be taken to design and optimize photonic crystal based spectrometers. The performance of these instruments are intimately linked to their F-number and the type of resonances inside the photonic crystals.

ACKNOWLEDGMENTS

The authors would like to thank Johannes Algera, Jochen Landgraf and Paul Tol for help on the atmosphere model and constructive discussion and feedback.

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