# Sensitivity analysis of a new SWIR-channel measuring tropospheric CH<sub>4</sub> and CO from space

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## ABSTRACT

In preparation for future atmospheric space missions a consortium of Dutch organizations is performing design studies on a nadir viewing grating-based imaging spectrometer using OMI and SCIAMACHY heritage. The spectrometer measures selected species (O<sub>3</sub>, NO<sub>2</sub>, HCHO, H<sub>2</sub>O, SO<sub>2</sub>, aerosols (optical depth, type and absorption index), CO and CH<sub>4</sub>) with sensitivity down to the Earth's surface, thus addressing science issues on air quality and climate. It includes 3 UV-VIS channels continuously covering the 270-490 nm range, a NIR-channel covering the 710-775 nm range, and a SWIR-channel covering the 2305-2385 nm range. This instrument concept is, named TROPOMI, part of the TRAQmission proposal to ESA in response to the Call for Earth Explorer Ideas 2005, and, named TROPI, part of the CAMEO-proposal prepared for the US NRC decadal study-call on Earth science and applications from space. The SWIR-channel is optional in the TROPOMI/TRAQ instrument and included as baseline in the TROPI/CAMEO instrument.

This paper focuses on derivation of the instrument requirements of the SWIR-channel by presenting the results of retrieval studies. Synthetic detector spectra are generated by the combination of a forward model and an instrument simulator that includes the properties of state-of-the-art detector technology. The synthetic spectra are input to the CO and CH<sub>4</sub> IMLM retrieval algorithm originally developed for SCIAMACHY. The required accuracy of the Level-2 SWIR data products defines the main instrument parameters like spectral resolution and sampling, telescope aperture, detector temperature, and optical bench temperature. The impact of selected calibration and retrieval errors on the Level-2 products has been characterized. The current status of the SWIR-channel optical design with its demanding requirements on ground-pixel size, spectral resolution, and signal-to-noise ratio will be presented.

Keywords: Optical Instrumentation, Remote Sensing, Space Technology, Troposphere, short-wave infrared, immersed grating, methane, carbon monoxide

# 1. INTRODUCTION

During the last couple of years the OMI and SCIAMACHY participating parties in the Netherlands, together with international partners, have been defining new mission concepts in order to prepare for the period after 2010, when SCIAMACHY<sup>1</sup> on ESA's ENVISAT and OMI<sup>2</sup> on NASA's EOS-Aura satellite have reached their end-of-life. The mission will benefit from the Dutch heritage that has been established by contributing to the design, building, and data analysis of the GOME (launched in 1995), SCIAMACHY (launched in 2002), OMI (launched in 2004), and GOME-2 (to be launched in summer 2006) instruments.

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The research objectives of the new mission are:

- to contribute to a better quantification and attribution of the sources and sinks of trace gases, including major greenhouse gases, short-lived precursor gases and aerosols on a global scale, and
- to contribute to a better understanding of the atmospheric transport, chemistry and radiation processes that drive the interactions between tropospheric composition, air quality and climate

The Dutch instrument contribution to such a mission will consist of a UV-VIS-NIR-SWIR nadir viewing grating-based spectrometer. The instrument will measure both the Earth radiance and solar irradiance spectra, in combination yielding the reflectance spectrum that contains the information for retrieval of atmospheric trace gases. The spectrometer includes 3 UV-VIS channels (270-490 nm), a NIR channel (710-775 nm), and a SWIR channel (2305-2385 nm). In order to improve with respect to the SCIAMACHY and OMI capabilities, the instrument has been designed with smaller ground pixels to increase the number of cloud-free observations and improved signal-to-noise performance. The instrument will measure the main tropospheric pollutants (O<sub>3</sub>, NO<sub>2</sub>, CO, CH<sub>2</sub>O and SO<sub>2</sub>) and two major climate gases (tropospheric O<sub>3</sub> and CH<sub>4</sub>). In addition, it will measure important parameters of aerosols (aerosol optical thickness, single scattering albedo, aerosol absorption index), which play a key role in tropospheric pollution as well as in climate change. Near-global daily coverage and unique diurnal time sampling with up to 5 daytime observations over midlatitude regions (Europe, North-America, China) is realized by using a non-sun-synchronous, medium-inclination drifting orbit.

The instrument concept has been proposed as TROPOMI, being part of the TRAQ mission in the framework of ESA's Earth Explorer Core Missions and as TROPI, being part of the CAMEO initiative proposed to the US National Research Council. TRAQ is selected by ESA – together with five other mission proposals - for a pre-phase A study. A subset of these six preselected mission candidates will be selected for phase A; the mission finally selected for implementation will be launched during the first half of the next decade. In addition, the instrument concept fits the recommendation of ESA's CAPACITY study to realize a LEO mission with a UV-VIS-NIR-SWIR nadir viewing spectrometer (GMES/Sentinel 5)<sup>3</sup>.

To continue and improve on the SCIAMACHY data record of CO and  $CH_4$  a SWIR channel is included in the design studies. This paper describes the derivation of the main instrument parameters for the TROPOMI and TROPI SWIR channels based on Level 2 CO and  $CH_4$  total column product requirements. An additional paper on the TROPOMI and TROPI instruments, in particular focusing on the UV-Vis-NIR channels, will appear in the proceedings of this conference as well<sup>4</sup>.

The paper is organized as follows: first, the main mission and Level 2 SWIR product requirements and the SWIR channel instrument concept are presented in section 2. Subsequently, the method for derivation of the instrument parameters using synthetic spectra is explained in section 3. The results of retrieval studies based on Monte Carlo simulations confine the main instrument parameters and are summarized in section 4. The status of the SWIR channel design is discussed in section 5. Conclusions and an outlook are provided in section 6.

## 2. THE TROPOMI & TROPI SWIR CHANNEL

The TROPOMI/TRAQ and TROPI/CAMEO SWIR channel roughly cover the 2.3-2.4 micron spectral range. In this spectral region the absorption spectrum is dominated by spectral features of  $CH_4$  and  $H_2O$ , and contains rather weak CO absorption lines. Back-scattered solar light in the SWIR spectral range reaches down to the Earth's surface, thus also probing the lowest parts of the troposphere.

#### 2.1. Level 2 product requirements

The derivation of the main instrument parameters for the TROPOMI and TROPI SWIR channel is based on the Level 2 CO and  $CH_4$  total column requirements<sup>5</sup>. Unless explicitly stated otherwise, the requirements mentioned here are valid for both the TROPOMI and TROPI instrument. General Level 2 product requirements relevant for CO and  $CH_4$  are:

- to attain (near-)global coverage within a couple of days at maximum
- sensitivity to the lowest kilometers of the troposphere and the planetary boundary layer
- to attain a horizontal resolution (nadir pixel)

- for TROPOMI in the 2 x 2 km<sup>2</sup> (target) to 10 x 10 km<sup>2</sup> (threshold) range. The requirement on ground pixel size is driven by the requirement for minimum cloud contamination, although the threshold pixel size of  $\sim 10 \times 10 \text{ km}^2$  is considered sufficient to address the research objectives. Only the threshold resolution is considered here, as for the SWIR channel the target requirements can not be realized using the proposed instrument concept.
- $\circ$  for TROPI of 20 x 20 km<sup>2</sup>
- to sample the CO diurnal cycle for air quality purposes. The high-revisit frequency of several observations per day is realized by the medium-inclination drifting orbit and is also driven by requirements on the UV-VIS air quality data products, in particular NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub>, and aerosols.

Three atmospheric scenes are defined: the minimum scene (surface albedo = 0.05, solar zenith angle (SZA) = 70) corresponding to mid- to high-latitude winter scenes as typical over Europe. The nominal scene (surface albedo = 0.2, SZA = 50) corresponds to a combination of moderately high surface albedo and a moderate SZA, and the maximum scene (surface albedo = 0.65, SZA = 10) to a bright mid-summer Sahara desert type scene. The requirements on Level 2 product accuracy are summarized in Table 1 and should also be met for the minimum scene.

Table 1. Level 2 SWIR product requirements.

Product	Accuracy	Units
CO (total column)	< 0.25	10 <sup>18</sup> molecules/cm <sup>2</sup>
CH <sub>4</sub> (total column)	< 2	%

## 2.2. SWIR-channel instrument concept

The OMI-technique involves push-broom imaging using 2D detector technology<sup>2</sup>. With this technique the complete swath is imaged along one direction of a 2D focal plane array (FPA), while the spectral information is projected along the other coordinate. To transfer the OMI 2D-imaging technology to the SWIR spectral domain while maintaining a compact instrument design, the use of immersed gratings<sup>6</sup> is mandatory. This technology is currently being made available to Dutch industry via a NL-nationally funded technology study. By immersing the grating groove pattern in IR materials with high refractive index, such as silicon (n=3.4) or germanium (n=4.1), the diffraction grating yields higher dispersion. As a consequence, the grating size, and thereby the SWIR spectrometer linear length, can be reduced by a factor corresponding to the refractive index of the immersion material compared to conventional echelle grating technology while providing the same spectral resolution. The associated reduction in volume and weight of the SWIR channel is more than one order of magnitude, thereby making the SWIR channel feasible for space applications.



Fig. 1 From left to right: interference contract microscope and scanning electron microscope images of grating structures on a silicon wafer, and a photograph of a silicon wafer with grating structures of varying line frequency and dimensions. (Courtesy of J.-J. Lankwarden and M. Bruyn, SRON)

In the immersed grating technology study several options are investigated: the use of germanium<sup>7</sup> or silicon<sup>8, 9</sup> as the immersion material; and for silicon low order or high order diffraction gratings. The most promising option is the high-order Silicon grating requiring "conventional" lithography techniques for grating pattern generation. Grating structures with frequencies up to 267 lines/mm have been produced on standard silicon wafers via this method. Production of

complete grating prisms either via processing of thick, monolithic silicon plates or via wafer bonding is in progress. Some preliminary results of grating structures imprinted on thin wafers are displayed in Fig. 1.

Detection of the spatial and spectral information is performed using state-of-the-art 2D hybrid FPAs employing HgCdTe as the photo-active material bonded to a CMOS read-out IC (ROIC).

## 3. METHOD FOR DERIVATION OF INSTRUMENT PARAMETERS

Retrieval studies using synthetic detector spectra have been performed to establish the main instrument requirements. The synthetic spectra are generated by using the Earth radiances produced by a forward model as input. An instrument simulator converts the radiance spectra to detector signals and determines the associated noise level based on the selected instrument configuration. The output of the instrument simulator is a set of synthetic spectra including noise that can be employed for Monte Carlo simulations. This set of spectra serves as input for the retrieval algorithm which extracts the total columns of CO and  $CH_4$ . More details on the forward model and instrument simulator are provided below.

## 3.1. Forward model

The forward model uses the US standard atmosphere in combination with the HITRAN 2004 spectroscopic database<sup>10</sup> to calculate the optical densities at the top of the atmosphere. The optical densities are converted to radiances using the Lambert-Beer law and a high-resolution ATMOS solar spectrum<sup>11</sup> (0.05 cm<sup>-1</sup>). More details on the forward model can be found in<sup>12-14</sup>. When aerosol scattering is included, a full line-by-line radiative transfer code including scattering is used to compute the top of the atmosphere radiance<sup>15, 16</sup>.

## 3.2. Instrument simulator

In order to derive the signal and noise levels, the photon flux to individual detector pixels is calculated based on the radiance spectrum that is provided by the forward model, which already takes the spectral resolution and sampling of the instrument into account. The photo-current generated in the individual detector pixels is calculated from the radiance spectrum taking the instantaneous field of view (IFOV), telescope aperture, transmission of the optical system, and detection efficiency into account.

To determine the signal-to-noise ratio (S/N) per ground pixel, noise contributions due to the atmospheric signal, dark signal (diode-leakage current and thermal background signal), read-out, and digitization, as well as the required coadding and binning factors are taken into account. The detector properties are based on currently available HgCdTe hybrid-CMOS FPAs with a ROIC containing a capacitive trans-impedance amplifier for each pixel, amongst others to obtain good linearity. Output of the instrument simulator is a set of 120 synthetic spectra that include realistic noise levels and is synthesized using the same atmospheric parameters but with different random noise values. In addition, calibration errors can be included in the synthetic spectra to establish detailed instrument and calibration requirements.

#### 3.3. Retrieval algorithm

The algorithm used to retrieve total CO and  $CH_4$  columns from the synthetic spectra is the Iterative Maximum Likelihood Method (IMLM) developed at SRON for retrieval of CO and  $CH_4$  total columns from SCIAMACHY's Channel 8<sup>12-14</sup>, which has been adapted to include the characteristics of the TROPOMI and TROPI instrument. The precision of the total column retrieval for CO and  $CH_4$  is determined as the standard deviation on the retrieved total columns obtained from the set of 120 synthetic spectra. The required accuracy on the CO and  $CH_4$  data products imposes upper limits on the retrieval precision, and thereby on the allowed noise level of the synthetic spectra. CO,  $CH_4$ , and  $H_2O$  total columns need to be retrieved simultaneously from the selected spectral region as their absorption lines strongly overlap in the 2.3-2.4 µm spectral region.

By determining their impact on the Level 2 SWIR products, the main instrument parameters (spatial resolution and sampling, spectral range and fit windows, S/N, effective telescope diameter, operational optical bench and detector temperature, binning factor, and integration time) are optimized to meet the Level 2 SWIR product requirements for a realistic instrument configuration.

## 4. RESULTS

#### 4.1. TROPOMI instrument parameters

First, only the instrument parameters for TROPOMI are presented, as in general the TROPOMI and TROPI SWIR channel instrument parameters are very similar. Subsequently, the differences between the TROPOMI and TROPI SWIR channel instrument parameters are discussed.

## 4.1.1. Main instrument requirements

The requirements on horizontal resolution and global coverage are met by combining a 10 km along-swath (nadir) ground pixel size with a 2600 km swath. Per detector pixel a 5 x 5 km ground pixel is sampled. The 10 km pixel size in the swath direction is realized by binning 2 pixels along the swath direction. The required number of detector pixels in the spatial direction is easily accommodated on currently available FPAs as the distortion of the telescope reduces the spatial sampling with increasing swath angle. The spatial resolution in the flight direction, determined by the combination of the focal length of the telescope and the slit, is 10 km. The integration time of 1.5 s is selected to match the spatial resolution in the flight direction.



Fig. 2. Retrieval precision of CO (left) and CH<sub>4</sub> (right) for the full-performance fit window as a function of spectral resolution for several oversampling rates. A low CO column of 10<sup>18</sup> molecules/cm<sup>2</sup> is used. The lower part of the figure shows the retrieval precision when only shot noise on the atmospheric signal is taken into account, while the upper part shows the retrieval precision when all noise sources are accounted for. Note the difference in vertical scales.

To determine instrument requirements on spectral range, resolution and sampling, retrieval simulations haven been performed for three different fit windows. Even though the accuracy requirements on the Level 2 total CO column product is more relaxed than for  $CH_4$ , CO drives the instrument requirements, as the spectral absorption features are

very weak. Selection of the fit window is therefore critical. The fit windows that have been tested are the 2350-2380 nm window containing the strongest lines of the CO *P*-branch, the 2324-2340 nm window containing the strongest lines of the CO *R*-branch, and the 2314-2375 nm window containing both CO branches, in the remainder of the article referred to as the full-performance fit window. The CO *P*-branch fit window provides by far the worst precision for CO retrieval, amongst others due to the fact that the CO *P*-branch absorption is weaker than the *R*-branch. This fit window is therefore disregarded in the remainder of this article. The full-performance window, containing the largest amount of spectral information, demonstrates the best retrieval precision. The precision of the retrieved  $CH_4$  total column for the full-performance fit window is more than a factor of two better than for the CO *R*-branch fit window under all conditions. For CO, the difference in retrieval precision between the two fit windows is less, up to a factor 1.6, due to the fact that the strongest CO absorption lines are already included in the CO *R*-branch fit window.

Fig. 2 shows the retrieval precision of CO and CH<sub>4</sub> total columns when using the full-performance fit window for the minimum scene as a function of spectral resolution and for several oversampling rates (defined as the ratio of spectral resolution and spectral sampling). Plots are provided both for the situation that only shot-noise on the atmospheric signal is taken into account (best possible performance, lower panels) and for the situation that all known noise sources are taken into account (upper panels). The scatter in the plots is dominated by the statistical noise in the Monte-Carlo simulations. The retrieval precision of CO, a molecule showing narrow absorption lines overlapping with CH<sub>4</sub> and H<sub>2</sub>O spectral features, clearly improves with improved spectral resolution when only shot noise on the atmospheric signal is taken into account. For CH<sub>4</sub>, dominating the spectrum and showing spectral features covering the complete wavelength range of interest, the effect is minimal. When the full noise calculation is considered, however, no apparent optimum for the spectral resolution are competing in the resolution range that is investigated. Increasing the oversampling factor results in a reduced retrieval precision due to an increased noise level, as is most obvious for CH<sub>4</sub> (upper right graph in Fig. 2). It can be concluded that for the minimum scene the retrieval precision for CO is close to the accuracy requirement, while for CH<sub>4</sub> the precision is far better than the Level 2 product accuracy requirement using the same set of instrument parameters.



Fig. 3. Individual signal (top left) and noise (bottom left) components for the minimum scene using the TROPOMI SWIR channel instrument requirements. The contributions of the atmospheric signal are shown in solid-gray, thermal background signal in dashed-black, diode-leakage current in dash-dot-black, digitization noise in dotted-black and read-noise in dashed-gray. The total signal and noise values are plotted in solid-black. Right: the corresponding S/N of the atmospheric spectrum, with a maximum of S/N = 93 at 2313 nm.

The spectral resolution of the SWIR channel is selected to be 0.25 nm, very similar to the spectral resolution of SCIAMACHY channel 8. The oversampling rate is 2, just meeting the Nyquist criterion, resulting in a spectral sampling

interval of 0.125 nm. This combination of moderately high spectral resolution and a low oversampling rate allows imaging of the complete full-performance fit window range on currently available CTIA-based high-performance FPAs.

The remainder of the main instrument requirements (effective telescope area, S/N, operational optical bench and detector temperatures) is derived in order to meet the Level 2 CO product requirements for the minimum scene and a low CO column of  $10^{18}$  molecules/cm<sup>2</sup>, while using the CO *R*-branch fit window.

The CO retrieval precision just meets the Level 2 product accuracy requirement for S/N (at 2313 nm)  $\geq$  93. The required S/N can be realized by selecting an effective telescope diameter of 2.4 mm, in combination with a detector temperature of 165 K and an optical bench temperature of 220 K. For these instrument parameters the individual signal and noise components, the total signal and noise values, and the achievable signal to noise ratio for the atmospheric signal (i.e. after correction for the dark signal) is presented in Fig. 3. From the top left panel it can be concluded that for the minimum scene the thermal background signal (blue) still exceeds the atmospheric signal (red). With proper calibration this should not be a problem, although it could be considered to further reduce the thermal background signal e.g. by spectral of spatial filtering or further reduction of the optical bench temperature. With the selected instrument parameters, the noise contributions of atmospheric signal, thermal background signal, read-noise, and the combination of diode-leakage current and Johnson noise are nicely balanced for the minimum scene, as can be concluded from the lower left panel; a coaddition factor of 2 is sufficient to avoid saturation of the detector full-well capacity even for the maximum scene. Table 2 summarizes the achievable S/N (at 2313 nm) and CO and CH<sub>4</sub> total column retrieval precisions with the selected TROPOMI SWIR channel instrument parameters for both the CO *R*-branch and full-performance fit window for the minimum, nominal, and maximum scenes.

Table 2. Achievable S/N for the minimum, nominal and maximum scene for the set of TROPOMI SWIR channel instrument parameters. Corresponding precisions on total columns of CO and CH<sub>4</sub> retrieval are included in the table both for the CO *R*-branch and the full-performance fit window.

Atm. scene	S/N	CO precision (10 <sup>18</sup> molecules/cm <sup>2</sup> )		CH <sub>4</sub> precision (%)	
		CO R-br.	Full perf.	CO R-br.	Full perf.
Minimum	95	0.27	0.19	1.3	0.50
Nominal	395	0.10	0.06	0.36	0.12
Maximum	1005	0.04	0.03	0.17	0.05

#### 4.1.2. Calibration accuracy requirements

The impact of errors on selected calibration parameters on the retrieved total CO and  $CH_4$  columns has been characterized to establish the requirements on the calibration accuracy. The calibration errors under consideration are:

- Offset: A wavelength and pixel number independent offset to the atmospheric spectrum, representative for an imperfect calibration of e.g. the analog offset. The offset is defined relative to the maximum radiance signal, and thus depends on the atmospheric scene.
- Spike, representative for example for a reduced response of a specific pixel in the spectrum. Central wavelength and amplitude of the spike are varied.
- Fast oscillation on continuum level, representative for e.g. etalon effects. The calibration error is modeled by multiplying the spectrum by a fast oscillating cosine-like function of varying amplitude and frequency.
- Slow variation on the continuum level, e.g. representative for non-perfect calibration of the drop-off in response at the edges of the spectral channel. The calibration error is modeled by multiplying the spectrum by a cosine-like shape (half a period) centered at the central wavelength, with a predefined amplitude
- Total Dark: A random, per pixel, error in the total dark signal (dark current signal plus thermal background signal) calibration. Magnitude expressed relative to mean total dark signal.
- Shift of the solar spectrum due to wavelength calibration error of the irradiance spectrum
- Shift of the absorption spectrum due to wavelength calibration error in the radiance spectrum



Fig. 4. Deviation of retrieved  $CH_4$  column with respect to the input column (top) and precision of  $CH_4$  retrieval (bottom) as a function of the magnitude of the offset calibration error (defined with respect to the maximum atmospheric signal level (at 2313 nm) in the SWIR channel spectral window).

For all calibrations parameters being investigated the allowed magnitude of the calibration error is calculated for both the CO R-branch and full-performance fit window. An example of the results of such a calculation is visualized in Fig. 4. The calculation is performed for  $CH_4$  and shows the deviation of the retrieved column with respect to the input column (top) and the precision of the retrieved column (bottom) as a function of the magnitude of the calibration error in the offset. The deviation to the input column shows a nearly linear dependence on the offset calibration error; the precision is clearly minimal when the offset calibration is perfect. It can be concluded that in general the calibration requirements for the full-performance fit window are less demanding than for the CO *R*-branch fit window, the only exceptions being the requirements on calibration of the offset and the shift of the absorption line spectrum.

#### 4.2. TROPI instrument parameters

Table 3. Main instrument parameters of the TROPOMI and TROPI SWIR channel.

Parameter	TROPOMI	TROPI
Viewing Geometry		
Platform height	720 km	1500 km
Swath	2600 km	2000 km
Across track spatial sampling	5 km	10 km
Along track spatial sampling	5 km	10 km
Across track binning factor	2	
Along track spatial resolution	10 km	20 km
Spectrometer parameters		
Effective telescope area	$4.52 \text{ mm}^2$	4.91 mm <sup>2</sup>
Spectral range	2305-2385 nm	
Full performance range	2314-2375 nm	
Spectral resolution	0.25 nm	
Spectral sampling	0.125 nm	
Optical bench temperature	220 K	
Detector parameters		
Quantum efficiency	80 %	
Detector temperature	165 K	
Integration time	1.5 s 1.74 s	

The TROPI instrument parameters, in general, are very similar to the TROPOMI instrument parameters. Here the parameters deviating from the TROPOMI SWIR channel are discussed: The CAMEO platform will be in a 1500 km altitude orbit. The TROPI SWIR channel swath angle is significantly reduced, resulting in a 2000 km swath, still providing near-global coverage within a few days. The requirement on horizontal resolution is a factor of two more relaxed than for TROPOMI, thus doubling the spatial resolution and sampling parameters. As a result, the IFOV per detector pixel is almost identical to the TROPOMI SWIR channel.

The integration time is 1.74 s, corresponding to 10 km ground track flight for a platform in a 1500 km altitude orbit. The 20 x 20 km<sup>2</sup> horizontal resolution of the TROPI SWIR channel is still a significant improvement compared to the SCIAMACHY channel 8 horizontal resolution of 30 x 120 km<sup>2</sup>. The achievable S/N and attainable precision of the retrieved CO and CH<sub>4</sub> total columns are very comparable to the TROPOMI SWIR channel performance. A summary of the key instrument parameters for the TROPOMI and TROPI SWIR channels is provided in Table 3. The corresponding performance of the TROPI SWIR channel is summarized in Table 4. The calculations to determine the calibration requirements have not been repeated yet for the TROPI SWIR channel. It is not expected, however, that the calibration requirements deviate considerably from the TROPOMI requirements.

Table 4. Achievable S/N for the minimum, nominal and maximum scene for the set of TROPI SWIR-channel instrument parameters. Corresponding retrieval precisions for CO and CH<sub>4</sub> total columns are included for both the CO R-branch and full-performance fit window.

Atm. scene	S/N	CO precision (10 <sup>18</sup> molecules/cm <sup>2</sup> )		CH <sub>4</sub> precision (%)	
		R-branch	Full perf.	<b>R-branch</b>	Full perf.
Minimum	102	0.22	0.18	1.1	0.52
Nominal	430	0.08	0.06	0.32	0.11
Maximum	1085	0.03	0.03	0.15	0.04

#### 4.3. Aerosols

The error on the retrieved  $CH_4$  and CO total columns introduced by aerosol scattering is investigated by including aerosol scattering in the calculation of the synthetic detector spectra, while excluding it in the retrieval itself, as has been performed previously to quantify the impact of aerosol scattering on  $CO_2$  total column retrieval<sup>16</sup>. The calculations are performed for several combinations of solar zenith angles, surface albedo, and aerosol optical thickness using the TROPOMI instrument concept only, although the results are expected to be very similar for the TROPI instrument. A (typical) CO column of 2  $10^{18}$  molecules/cm<sup>2</sup> is used. The calculations are performed for four different types of aerosols: dust, marine, sulfate, and soot, representative for desert sites, the oceans, the industrial areas, and biomassburning regions, respectively. As the accuracy requirement on the Level 2  $CH_4$  product is very demanding, the effect of aerosol scattering on the retrieved total columns is most critical for  $CH_4$ . In general, the effect of aerosol scattering on the CO column accuracy is small compared to the required accuracy.

Preliminary results show that the Level 2 product accuracy requirements for  $CH_4$  (2%) are not met under the following conditions:

- Low surface albedo (<0.05) in combination with high SZA (60-70 degrees), and high Aerosol Optical Thickness (AOT) (>0.5) soot and sulfate aerosols
- High surface albedo (>0.3) and high AOT (>0.5) dust particles (as typical for sand storms at desert sites)

To meet the requirements under these conditions as well, either additional light path information should be available, or the properties of aerosols (type, size distribution, optical depth, height distribution) should be known for the location and time at which the trace gas measurements are performed to allow a first order correction of the scattering effect. This information will be provided by measurements in other wavelength ranges, for example the from the NIR  $O_2$  Aband channel. For the TRAQ mission the OCAPI instrument, present on the same platform, will be providing essential and unique information on tropospheric aerosols.

#### 5. OPTICAL, THERMAL, AND MECHANICAL DESIGN

Preliminary optical design studies on the TROPOMI SWIR channel have been performed, including specification of the required immersed grating. The details of the optical design of the SWIR channel depend on the type of immersed grating that is employed. The optical design must allow implementation of a polarization scrambler to reduce the complexity of the radiometric calibration, as is successfully used for the UV-VIS channels in OMI<sup>17</sup>. A trade-off taking the feasibility, advantages and disadvantages (amongst others the potential introduction of spectral features and a reduced spatial resolution) of a polarization scrambler in the SWIR spectral range into account will be performed in the near future.



Fig. 5. Mechanical layout of the TROPOMI SWIR module, also showing the detector module (left) and field-of view (top).

A preliminary design of the mechanical layout of the TROPOMI SWIR channel module is visualized in Fig. 5. A challenging aspect of the thermal-mechanical design is the fact that the medium-inclination drifting orbit requires regular yaw-flip maneuvers each time the solar elevation angle becomes negative (in practice almost every 5 weeks). The maneuver guarantees that the radiative cooler, cooling the instrument and FPAs, is permanently kept under cold conditions. The drifting orbit requires an observation strategy for solar irradiance measurements that differs from those defined for instruments in sun-synchronous orbits, like SCIAMACHY and OMI. Currently several optical designs for measuring the solar irradiance are under studyThe SWIR module has an estimated mass of ~35 kg, and a volume of ~40 liter, the radiative cooler (not shown in Fig. 5) included, and a power consumption of between 15W (nominal) and 70 W (peak).

## 6. CONCLUSIONS AND FUTURE WORK

The set of instrument and calibration parameters for the TROPOMI/TRAQ and TROPI/CAMEO SWIR channel is derived based on the Level 2 SWIR product requirements. Retrieval studies indicate that the OMI-concept can be successfully applied in the SWIR spectral range as well.

The SWIR channel key instrument requirements are predominantly determined by the required accuracy of the CO total column product which should be met even for the minimum scene. With the selected set of instrument requirements the precision of the  $CH_4$  total column easily exceeds the Level 2 product accuracy requirements. The accuracy of the  $CH_4$  total column is dominated by biases, such as the bias introduced by aerosol scattering, rather than the precision of the retrieval. The combination of immersed grating technology and state-of-the-art HgCdTe hybrid CMOS detector technology make the SWIR module the most innovative part of the TROPOMI instrument.

Future work focuses on continued development and manufacturing of the optimal immersed grating. The optical design will be adjusted to the outcome of this development, and will be extended to include the calibration options for solar irradiance measurements, white-light-source measurements and detector calibration.

In the near future a bread board model SWIR channel combining the most essential elements, the immersed grating, the SWIR polarization scrambler, and a hybrid CMOS FPA, will be developed to demonstrate technology readiness,

functionality, and performance by recording gas cell absorption measurements on  $CH_4$  and CO in the 2.3-2.4 micron spectral range.

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