General response to reviewer 4
We have responded to each of your points below, with your text in red and ours in blue.

You identified a number of areas where we did not provide enough information for easy replication, and also a number of areas where we did not provide enough context or emphasise key points of interest for more general readers. Our changes have addressed all of your points and your incisive comments greatly improved the paper. Thank you for your time.

In some cases we struggled between clarity and providing details but have found a balance. For example, we use 12 μm for r_{eff} based on the mean of the full PDF that is fit to MODIS data being 12.0 μm, but after applying thresholds the mean shifts to 12.6 μm, explaining some apparent differences in our original submission. We have added explanatory text where necessary.

Our updated introduction and Figure 6 combine to tell a nice story: OCO-2 has sufficient spectral resolution to retrieve geometric thickness, given our assumptions and based on previous work which we now describe in more detail. MERIS or even GOME-2 do not, and our new Figure 6 shows a GOME-2-like calculation where we replicate previous work by Schuessler et al. Multi-angular measurements should retrieve thickness, but only for geometrically thick clouds (multi-km+), so OCO-2 is complementary to them.

Other instruments have high spectral resolution so the results may carry over, and we list those of which we are aware (TROPOMI on Sentinel-5P, the spectrometers on the FengYun-3 series and GOSAT). We also point out where spatial resolutions differ (OCO-2 is better than TROPOMI/GOSAT), but also that OCO-2's narrow swath is a limitation compared with TROPOMI's much better coverage.

Changes made based on your comments, and those of the other reviewers, have made us provide much more context and resulted in a richer narrative that we hope will make the paper far easier to read and more widely useful. Thanks once again.

NOTE: our page and line numbers refer to the new version. With our greatly expanded introduction and other minor corrections it became very messy otherwise. Also note that we have added a new Figure 6, which is appended to the end of this document. In addition, the full new introduction follows the figure.

Interactive comment on "Information content of OCO-2 oxygen A-band channels for retrieving marine liquid cloud properties" by Mark Richardson and Graeme L. Stephens

Anonymous Referee #4

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This paper analyzed the information content in O2 A band for retrieving marine liquid cloud properties. it used the Rodgers (2000) formal optimization framework and expressed the information content in terms of degree of freedom for signal and Shannon entropy. The O2 A band on OCO-2 has 800+ channels, and this paper shows that only _75 channels are needed to retain all information content for retrieving cloud optical depth, cloud pressure thickness, and cloud-top pressure. The method in this paper is sound, but revisions are needed to include various advances in recent studies of using O2 A and B for cloud/aerosol height retrievals, as well as more justification about assumptions and caveats in this study.

1. Abstract. what is cloud-pressure thickness? what is the unit here?

- ➔ **Response:**
- ➔ **Changes made:** Abstract changed: "…and cloud-pressure thickness, which is the geometric thickness expressed in hPa."

2. Introduction. Most references cited in the first paragraph are theoretic work done in the past. While they are interesting, there are renewed interests in recent years to use O2 A and B band to retrieve cloud/aerosol height, with some using real data with good validations. They should be included in this paper, and discussion should be made that recent studies with real data use only O2 A/B bands from an

imager (such as EPIC or MERES), although some studies did recommend the use of spectra to retrieve aerosol height. See references below and references therein (including some work done by authors' colleagues in JPL).

Ding, S. et al., 2016, Polarimetric remote sensing in O2 A and B bands: Sensitivity study and information content analysis for vertical profile of aerosols, Atmospheric Measurement Techniques, 9, 2077-2092.
Xu, X. et al., 2017, Passive remote sensing of altitude and optical depth of dust plumes using the oxygen A and B bands: First results from EPIC/DSCOVR at Lagrange-1 point, Geophys. Res. Lett., 44, 7544-7554.

- ➔ **Response:** We chose to be brief and limit discussion to things relevant to our hyperspectral result, but agree that we sliced out too much contextual work. Our changes were made to address all reviewers and we decided to focus on the cloud-relevant components. We reference Yang et al. (2013) for EPIC/DSCOVR since they looked at clouds. We add Ding et al. later in the text (see comment 5).
- ➔ **Changes made:** The introduction has been rewritten and substantially lengthened with citations to Hanel (1961), Yamamoto & Wark (1961), Deschamps et al. (1994), Ferlay et al. (2010), Desmons et al. (2013), Merlin et al. (2016), Yang et al. (2013), Rozanov & Kokhanovsky (2004), Schuessler et al. (2014), Heidinger & Stephens (2000) and O'Brien & Mitchell (1992). These support a new summary of various A-band cloud studies and then justify our new work as applying hyperspectral approaches that are useful for low clouds. We cite Bony & Dufresne (2005) and Zelinka et al. (2012) to support the importance of low clouds that are poorly sampled by the multi-angular approaches, and explain our advantages for geometrical thickness relative to other work that used instruments with lower SNR and spectral resolution.

3. Section 2. It should be made clear if cloud properties are well characterized, will CO_2 be retrieved accurately in cloudy-sky conditions? If so, is it column CO_2 above cloud top or whole atmospheric column, including CO_2 within cloud? Any references will be helpful in this regard. To what degree of accuracy of cloud properties are needed in order to retrieve CO_2 with good accuracy?

- ➔ **Response:** Our current retrieval will not allow this because we do not retrieve droplet effective radius, and droplet radius is needed since the wavelength differences between the O_2 band and CO_2 bands is large enough that it matters for the XCO_2 retrieval. We now cite a paper whose figure shows that not knowing the droplet size causes a ~15 ppm spread in above-cloud CO_2 retrievals, which is far larger than the <1 ppm that are reported as the requirements for the flux modellers.
- ➔ **Changes made:** p3L30—p3L24 now reads: "This approach aims to optimise a cloud property retrieval and due to limitations related to the radiative transfer implementation and computational burden, droplet size is not a retrieved property but contributes to the posterior uncertainty. Above-cloud CO_2 retrievals have been found to require cloud droplet size for good accuracy (Vidot et al., 2009) and therefore our current implementation will not directly lead to above-cloud CO_2 retrievals."

4. Section 2.1. It is noted that there are often aerosol layer above marine boundary layer cloud. To be clear, no aerosol effects are treated in L2RTM, correcT? How about surface reflectance?

- ➔ **Response:** We have had some issues properly integrating aerosols into the cloudy-scene L2RTM, although the operational "clear sky" XCO_2 retrieval run for the OCO-2 mission allows for optically thin layers of stratospheric aerosols. We have added text to emphasise the limitations and that this is future work. We also realise that the surface requires further explanation. We now describe our surface model.
- ➔ **Changes made:** Regarding the surface, p3L32—p4L2 now reads: "Water surfaces at nadir are dark, and even in cloud-free cases there is rarely sufficient SNR for the OCO-2 algorithm to attempt an XCO_2 retrieval. We assume a Cox-Munk surface reflectance function with the L2RTM surface reflectance set to 0.10, but as we only use nadir view over ocean there is little sensitivity to surface properties."

- ➔ Regarding aerosols, p3L10—12 now reads: "Our current analysis considers aerosol-free cases as aerosols have not yet been properly implemented in our modified cloudy-sky version of the radiative transfer model, this is an avenue for future work and will be discussed in Sect. 5."

  P13L32—p14L9 now reads: "Alternatively, since OCO-2 flies in the A-train it would also be possible to use other sensors such as CALIPSO (which is now leaving the A-train) or MODIS to identify multi-layer cloud cases, or scenes in which there is heavy aerosol loading. Cases of heavy aerosol loading are most common over the Namibian stratocumulus region with common occurrence in June-July-August (JJA) and a peak in September-October-November (SON). A combination of CALIPSO, CloudSat and International Satellite Cloud Climatology Project (ISCCP) data imply that in the SON Namibian stratocumulus region, approximately one-third of low clouds have overlying aerosol, and approximately half of these cases are smoke (Devasthale and Thomas, 2011; Winker et al., 2010). Scattering layers overlying a marine cloud tend to reduce in the effective retrieved cloud layer pressure due to the reduced mean path length of those photons reflected from the overlying layer (Vanbauce et al., 1998). Assessment of aerosol effects will be necessary in future work."

section 2.2. what is the state vector? optical depth, top pressure/height? be clear here. This also applies to the title of this paper. what properties to be retrieved? droplet size, top pressure/height or optical depth?

- ➔ **Response:**
- ➔ **Changes made:** p6L4—p6L6 now reads: "We follow the principles of optimal estimation from (Rodgers, 2000), where a Bayesian retrieval combines an observation vector y with a prior state vector x_a and obtains a posterior state x ̂. In our case the state vector consists of cloud-top pressure P_top, cloud pressure thickness ΔP_c and cloud optical depth τ."

5. Page 4, Line 25. Ding et al. (2016) used similar method to select channels needed in O2 A and B band for aerosol retrievals. It is worthy to mention here.

- ➔ **Response:**
- ➔ **Changes made:** Text added: "…(Chang et al., 2017; Mahfouf et al., 2015; Martinet et al., 2014; Rabier et al., 2002), and this approach has already been used in an oxygen A-band and B-band analysis for aerosol retrievals (Ding et al., 2016)."

6. Page 5, L20. How about effective variance of cloud droplet size? Does it matter?

- ➔ **Response:** See response to comment 8.
- ➔ **Changes made:**

7. Page 6, L2. "A pressure scale height of 8 km is assumed to convert the resultant....". This sentence is hard to comprehend.

- ➔ **Response:**
- ➔ **Changes made:** text re-written as "Cloud geometric thickness is converted to pressure thickness by assuming that pressure decreases exponentially with altitude with a scale height of 8 km"

8. Page 6, L27. mean of 12.6 um? should it be 12 um to be consistent with previously stated? How about effective variance?

- ➔ **Response:** With our modified L2FP code we have to select integer values of reff and picked a value close to the peak (the exact value depends on the statistic you use: arithmetic mean is 12.6 microns but you can get other values from a log fit, taking the median, mode or others). We have mentioned the integer sampling earlier in the text, but think that adding extra text here is clunky so have made no changes. We have, however, added clarification text where we think it does not interrupt the flow.
- ➔ **Changes made:** p5L29—p5L32 now reads: "Mie scattering computations are used within louds using relevant coefficients that are pre-calculated for gamma distributions of cloud droplets based on a summary of low-cloud studies (Miles et al., 2000). These values have only been pre-computed for integer values of effective droplet size. This should not affect our results greatly since our calculated uncertainties include a term spanning a range of droplet sizes."

  P11L4—o117 now reads: "The r_eff distribution effective variance is fixed in each case in order to use the pre-calculated scattering properties used with the L2RTM code, but given the wide range of effective mean values considered, it is not expected that allowing the effective variance to change would greatly affect the results."

9. Page 6, L29. cloud top pressure of 850 hpa? but, in the 3.1, it says three different pressures.

- ➔ **Response:** We calculated covariance calculations for a single cloud-top pressure but used multiple cloud-top pressures in the calculation of information content and in the synthetic retrievals to more effectively use compute time. Our posterior sample spread from the synthetic retrievals therefore includes any uncertainty introduced by calculating the covariances at a single ctP.
- ➔ **Changes made:** p9L9—p9L11 now reads: ". We calculate covariances at a single value of P_top, but the convergence of our synthetic retrieval tests across a range of true P_top values shows that we obtain reliable results regardless."

10. Page 8, L10. what is the priori for cloud top pressure here? what is the error in OCO-2 measurement itself?

- ➔ **Response:** Clarification text added. We had provided information on the Ptop apriori but not the specific instrumental uncertainty relevant to these values. We have repeated the Ptop prior details so that hopefully readers don't miss them.
- ➔ **Changes made:** p10L25—p11L2 now reads: "The squared OCO-2 radiance uncertainties are added to the diagonal elements of the observation error covariance matrix with no cross correlation. We use the standard OCO-2 version 7 uncertainties, and SNR increases as the radiance in a given channel increases. The median SNR ranges from just over 400 for the $\tau = 5$ cases to around 700 for the $\tau = 25$ cases. The SNR reaches a minimum of 72 in an absorption band channel in a $\tau = 5$ case, and a maximum of 763 in a weakly absorbing channel in a $\tau = 25$ case.

  Forty true cloud cases are used with five of each case where optical depth ranges from 5 to 40 in increments of 5 and cloud-top pressure is randomly selected to be between 680—900 hPa and rounded to the nearest 10 hPa. The prior cloud properties are assumed to be unbiased, so are randomly sampled from a Gaussian with a mean equal to the truth and a standard deviation equal to the prior errors above. Each synthetic retrieval begins with a separate prior, and the prior is also used as the first guess."

11. P10, L7. Do these 75 channels have the same wavelenghts for all test cases?

- ➔ **Response:** Yes, text added and we have added reminders and clarifications throughout. You're right that this is an important point!
- ➔ **Changes made:** p5L6 text added: "but will select a consistent micro-window of the same channels for each."

  P10L13—p10L15 now reads: "While this may result in a different location for each size of micro-window, the location is fixed for an individual case, i.e. the 5-channel microwindow consists of the same 5 channels in all 216 cases."

  P12L18—p12L20 reads: "the 75 channel micro-window containing the OCO-2 channels 353—426 (indices counting from 1 for the full 1,016 OCO-2 L1bSc channels) consistently satisfies our P_top and ΔP_c criteria and reduces the full wavelength range from 759.2—771.8 nm to 763.5—764.6 nm." [inclusion of channel indices helps imply it's fixed]

  New Figure 6 shows the selected channels.

12. P11, last sentence. what is proposed here is a strong statement. What is the basis to support that "assumptions made here don't affect primary conclusion" here?

- ➔ **Response:** Fair point
- ➔ **Changes made:** Text removed.

13. Finally, it is not all that clear if measurement in O2 A with such a finer spectral resolution will be needed? In other words, using 75 channels vs. using just one channel (such as from EPIC, MERES or TROPOMI) for cloud retrievals, are there huge differences? Answering this question will greatly improve the impact of this paper.

- ➔ **Response:** We now report the spectral resolution requirements given by O'Brien & Mitchell and Heidinger & Stephens. We also reproduced a calculation similar to Schuessler et al. and get the same answer: that GOME-2 spectral resolution isn't enough to obtain the three pieces of information we require. Our expanded introduction now explains that two A-band channels are insufficient (implicitly addressing MERIS, though we use POLDER as an example). We also now discuss TROPOMI – it has the nominal spectral resolution, its larger spatial resolution will be a disadvantage in heterogeneous scenes however.

➔ **Changes made:** p2L29—p2L30 text added: "However, older theoretical work suggested that a spectral resolution of better than 1 cm-1 (O'Brien and Mitchell, 1992) or even 0.5 cm-1 (Heidinger and Stephens, 2000) is required for an effective A-band retrieval that includes cloud geometric thickness."

New Figure 6 and p12L21—p12L28 text added: "Figure 6 shows an example cloudy scene spectrum simulated for OCO-2 and highlights the chosen 75 channel micro-window in red. Also shown is an approximated GOME-2 spectrum based on the MetOp-B instrument characteristics (Munro et al., 2016). We approximate the ILS using Gaussian instrument line shapes, taking the 0.21 nm spectral sampling from Table 1 and FWHM of 0.50 nm from Table 2 of Munro et al. (2016). While OCO-2 spectra allow 3 independent pieces of information to be obtained (see the reported d_s in the figure caption) our calculations agree with previous work that the GOME-2 resolution only provides approximately 2 (Schuessler et al., 2014). Consistent with older theoretical work (Heidinger and Stephens, 2000; O'Brien and Mitchell, 1992) this analysis supports the case that OCO-2's high spectral resolution leads to additional information about cloud geometric thickness."

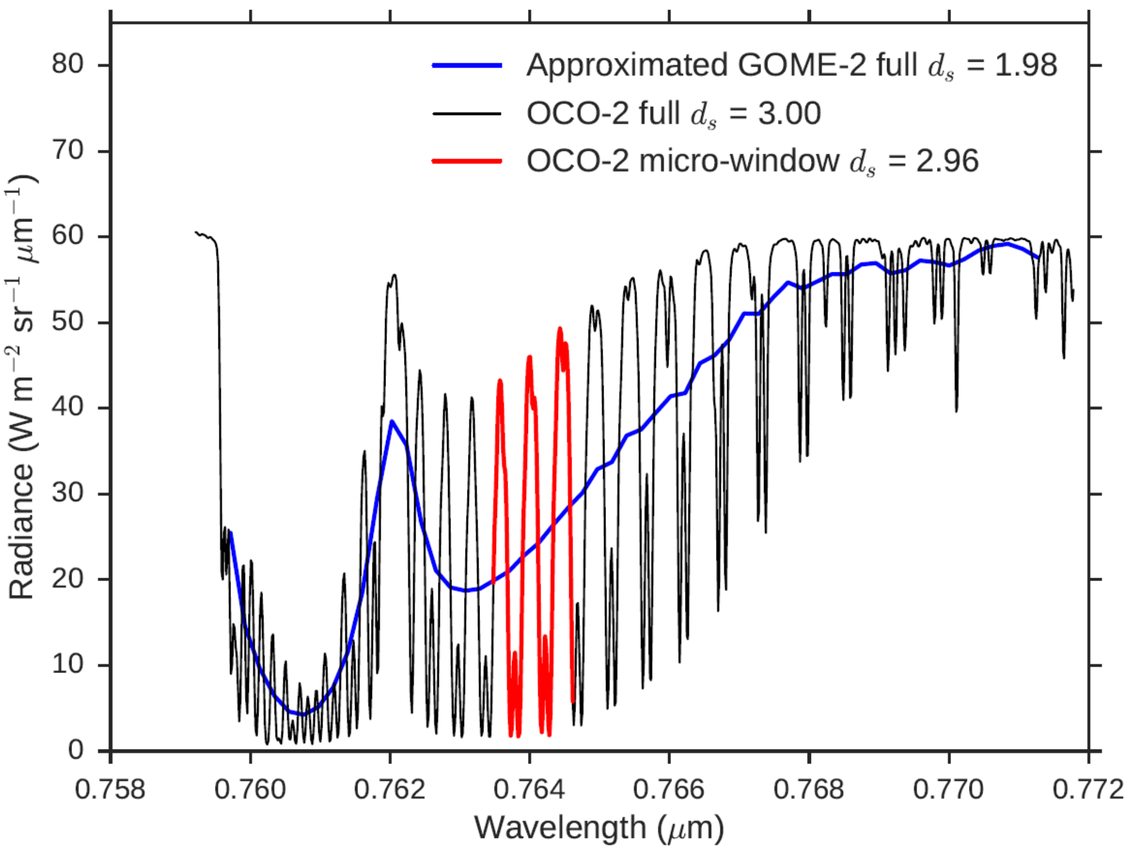

Figure 1 Example simulated cloudy scene A-band spectrum, for a τ = 10, P_{top} = 850 hPa cloud in a tropical atmosphere with a solar zenith angle of 45°. The black line shows the full OCO-2 simulated spectrum, the blue line is the black line resampled using approximate GOME-2 instrument line shapes and the red line is the selected 75 channel micro-window

for OCO-2 cloud retrievals. The legend also reports the d_s for each spectrum with the GOME-2 instrumental uncertainty based on an SNR of 100 as in previous work (Schuessler et al., 2014).

FULL NEW INTRODUCTION:

The oxygen A-band spans wavelengths with a wide range of absorption strength which can be exploited to determine photon path lengths and therefore retrieve cloud top heights and potentially the within-cloud photon path, which is related to droplet number concentration and therefore cloud thickness. Meanwhile, cloud optical depth can be retrieved from reflectance in approximately non-absorbing "continuum" channels (Fischer and Grassl, 1991a; Koelemeijer et al., 2001; Stephens and Heidinger, 2000). Such a retrieval that includes cloud geometric thickness or droplet number density would allow evaluation of model cloud physics (Bennartz, 2007). In addition A-band retrievals use reflected sunlight so are physically independent from other common sources of cloud information such as longer wavelength infrared, which may mis-identify cloud-top pressure in the presence of temperature inversions (Baum et al., 2012).

The photon path length of reflected sunlight is estimated by comparing radiance between channels with different absorption characteristics. With known absorption coefficients and similar scattering and reflection properties between the channels, the photon path length is easily determined from the Beer-Lambert Law. This technique was first suggested as a way of determining cloud-top altitude using the strong carbon dioxide (CO_2) absorption band near 2.0 μm with an atmospheric window near 2.1 μm (Hanel, 1961). Subsequently the oxygen A-band near 0.76 μm was proposed as it offers improved signal to noise (SNR) and avoids overlap with the 1.87 μm water vapour absorption band (Yamamoto and Wark, 1961). It was noted that clouds are not "simple diffuse reflectors" and that "absorption along the scattering paths within the clouds must be considered".

With a single measured ratio of two channels it is only possible to determine the total photon path length and not distinguish between above-cloud and within-cloud components, as this would mean obtaining two pieces of information from a single measurement. One way of distinguishing is to take multiple measurements from diverse viewing angles, as is done by the Polarization and Directionality of the Earth's Reflectances (POLDER) instrument series (Deschamps et al., 1994). POLDER-3 has a "narrow" channel with a full width at half maximum (FWHM) of 10 nm centred at λ = 763nm, and a "wide" channel of FWHM 40 nm centred at 765 nm. Statistics of the inferred photon path from different angles have been shown to be related to the cloud centroid pressure (Ferlay et al., 2010), results of which have been tested against CloudSat radar and Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO) data (Desmons et al., 2013). A more recent study used an information content analysis based around the characteristics of the Multiviewing, Multi-channel and Multi-polarization Imaging (3MI) and the Multiangle SpectroPolarimetric Imager (MSPI) instruments. This concluded that multiangle measurements are informative about cloud geometric thickness, particularly for clouds thicker than 2—3 km (Merlin et al., 2016), which notably excludes the marine stratocumulus regime.

Another proposal to obtain additional measurements that inform about cloud geometric thickness is to combine measurements from both the oxygen A-band and B-band, such as those available from the Earth Polychromatic Imaging Camera (EPIC) on the Deep Space Climate Observatory (DSCOVR). By considering the sum and differences of the channel ratios it has been proposed that cloud geometrical thickness can be retrieved when cloud optical depth (τ) is greater than 5 (Yang et al., 2013).

An alternative to multiple angles or additional bands is to measure more channels in the A-band, as was done for the Scanning Imaging Absorption SpectroMeter for Atmospheric Chartography (SCIAMACHY) on board ENVISAT (Rozanov and Kokhanovsky, 2004), which when combined with the Global Ozone Monitoring Experiment instruments (GOME and GOME-2), provide an A-band record since 1995. An information content analysis based on GOME-2 characteristics, using a spectral resolution of 0.2 nm and assumed signal-to-noise (SNR) of 100 showed that 2 pieces of information could be obtained (Schuessler et al., 2014). This study showed the best performance when retrieving cloud-top height with either τ or cloud fraction and reported that there was not sufficient information in these assumed measurements to obtain cloud geometric thickness with "satisfactory accuracy",

However, older theoretical work suggested that a spectral resolution of better than 1 cm^{-1} (O'Brien and Mitchell, 1992) or even 0.5 cm^{-1} (Heidinger and Stephens, 2000) is required for an effective A-band retrieval that includes cloud geometric thickness. In wavelength terms this is 0.03—0.06 nm, and is now achieved by instruments carried by the Chinese Feng-Yun 3 series (most recently FY-3D), the Japanese Greenhouse Gas Observing Satellite (GOSAT), the European Sentinel-5 Precursor (Sentinel-5P, which carries the Troposphere Measuring Instrument "TROPOMI") and NASA's Orbiting Carbon Observatory-2 (OCO-2).

This study considers OCO-2 and extends previous work that developed a lookup table to retrieve cloud-top pressure and optical depth for single layer liquid clouds over ocean (Richardson et al., 2017). This simple retrieval combined 20 of OCO-2's 853 functioning A-band channels into 2 "super-pixels" or "super-channels" based on their O_2 absorption. The lookup tables were used for all locations and weather conditions and were validated using collocated Moderate-resolution Imaging Spectroradiometer (MODIS) and CALIPSO data (Taylor et al., 2016). Here we develop an optimal-estimation-based retrieval (Rodgers, 2000) for single-layer water clouds over oceans using nadir-view OCO-2 measurements and subject it to several idealised tests. This study's new contributions are (i) considering information content aspects to select groups of channels rather than combined super-channels, (ii) accounting for local meteorological conditions and (iii) adding cloud pressure thickness to the retrieved state. We express cloud geometric thickness in terms of hPa and refer to it as cloud pressure thickness with the symbol ΔP_c. Our current analysis considers aerosol-free cases as aerosols have not yet been properly implemented in our modified cloudy-sky version of the radiative transfer model, this is an avenue for future work and will be discussed in Sect. 5.

OCO-2 has 1,016 A-band channels of which 853 function across all soundings with spectral sampling between 0.01—0.02 nm and a FWHM of 0.04 nm in wavelength, implying sufficient spectral resolution for geometric thickness retrievals. Low marine clouds are the primary cause of spread in net modelled cloud feedback (Bony and Dufresne, 2005; Zelinka et al., 2012) and we focus on these clouds, which complements the multi-angular retrievals from other sensors which appear to perform better for thicker clouds (Ferlay et al., 2010; Merlin et al., 2016).

OCO-2 is also promising as its SNR values commonly range from 300—800 in cloudy scenes and it flies in the A-train constellation (L'Ecuyer and Jiang, 2010), allowing collocation with other sensors. Furthermore, its footprint size typically ranges from 1.2—2.3 km at nadir and compares favourably with both GOSAT (10.5 km diameter) and TROPOMI (7×7 km^2), although its narrow swath of approximately 10 km is much reduced compared with TROPOMI's 2600 km.

Here we aim to develop a computationally efficient cloud retrieval for OCO-2 by selecting channels that contain the most information about the retrieved state properties, which speeds both the radiative transfer simulation and the optimal estimation calculations. In principle, the optimal channels may depend on the cloud case and on the across-track position of the measurement because the instrument line shapes (ILS) vary across the swath. Furthermore, neighbouring ILS overlap so it is more computationally efficient to select neighbouring channels since the radiative transfer will already have been calculated for many of the relevant frequencies. We refer to the selection of neighbouring channels as a "micro-window" approach and use the OCO-2 Level 2 Full Physics Radiative Transfer Model (L2FP RTM, (Boesch et al., 2015)) with a set of representative atmosphere and liquid cloud states to select the optimal micro window based on information content and posterior error criteria.

This approach aims to optimise a cloud property retrieval and due to limitations related to the radiative transfer implementation and computational burden, droplet size is not a retrieved property but contributes to the posterior uncertainty. Above-cloud CO_2 retrievals have been found to require cloud droplet size for good accuracy (Vidot et al., 2009) and therefore our current implementation will not directly lead to above-cloud CO_2 retrievals.

The paper is organised as follows: Sect. 2 describes the OCO-2 satellite measurements, radiative transfer model and general information content approach. Sect. 3 details the methodology specific to this paper, including the sample atmospheres, perturbations for determining covariance matrix components, the sequential channel selection procedure and information content and retrieval analysis. Sect. 4 reports the results of each of these cases, Sect. 5 discusses the results and describes how they will be applied in the real OCO-2 cloud retrieval, and Sect. 6 concludes.