

Abstract

Since the launch of the Greenhouse Gases Observing Satellite (GOSAT) in 2009, retrieval algorithms designed to infer the column-averaged dry-air mole fraction of carbon dioxide (X_{CO_2}) from hyperspectral near-infrared observations of reflected sunlight have been greatly improved. They now generally include the scattering effects of clouds and aerosols, as early work found that absorption-only retrievals, which neglected these effects, often incurred unacceptably large errors, even for scenes with optically thin cloud or aerosol layers. However, these “full-physics” retrievals tend to be computationally expensive and may incur biases from trying to deduce the properties of clouds and aerosols when there are none present. Additionally, algorithms are now available that can quickly and effectively identify and remove most scenes in which cloud or aerosol scattering plays a significant role.

In this work, we test the hypothesis that non-scattering, or “clear-sky”, retrievals may perform as well as full-physics retrievals for sufficiently clear scenes. Clear-sky retrievals could potentially avoid errors and biases brought about by trying to infer properties of clouds and aerosols when none are present. Clear-sky retrievals are also desirable because they are orders of magnitude faster than full-physics retrievals. Here we use a simplified version of the Atmospheric Carbon Observations from Space (ACOS) X_{CO_2} retrieval algorithm that does not include the scattering and absorption effects of clouds or aerosols. It was found that for simulated Orbiting Carbon Observatory-2 (OCO-2) measurements, the clear-sky retrieval had errors comparable to those of the full-physics retrieval. For real GOSAT data, the clear-sky retrieval had nearly indistinguishable error characteristics over land, but roughly 30–60 % larger errors over ocean, depending on filtration level, compared to the full-physics retrieval. In general, the clear-sky retrieval had X_{CO_2} root-mean-square (RMS) errors of less than 2.0 ppm when adequately filtered through the use of the Data Ordering through Genetic Optimization (DOGO) system. These results imply that non-scattering X_{CO_2} retrievals are potentially much more accurate than previous literature suggests, when employing fil-

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tering methods to remove measurements in which scattering can cause significant errors. Additionally, the computational benefits of non-scattering retrievals means they may be useful for certain applications that require large amounts of data but have less stringent error requirements.

1 Introduction

Recently, space-based instruments such as the Greenhouse Gases Observing Satellite (GOSAT; Yokota et al., 2009) and the Orbiting Carbon Observatory-2 (OCO-2; Crisp et al., 2008) have been launched with the goal of providing accurate global measurements of greenhouse gas concentrations, including carbon dioxide (CO₂). Only approximately half of the anthropogenically emitted CO₂ stays in the atmosphere. The remaining molecules are absorbed by the land and ocean, but where this absorption takes place is still highly uncertain, especially over land surfaces (Le Quéré et al., 2009). Carbon flux models, designed to answer important questions about Earth's carbon sources and sinks and their interaction with the atmosphere, are heavily dependent on the density and quality of CO₂ measurements (Rayner and O'Brien, 2001; Baker et al., 2010; Chevallier et al., 2007, 2009). Global coverage of CO₂ measurements will improve the accuracy of their results, but only if the space-based measurements are of sufficiently high accuracy themselves. Specifically, it has been shown that a precision of better than about 0.5 % (~ 2 ppm for CO₂) for space-based measurements is needed to gain more information about the carbon cycle compared to only having access to ground-based measurements (Miller et al., 2007). In terms of a bias between the measured CO₂ and the true amount present in the atmosphere, even a regional bias of a few tenths of a ppm may be detrimental to carbon flux models (Chevallier et al., 2007; Basu et al., 2013). Thus, it is critically important to minimize errors and biases in satellite measurements of CO₂ in order to be able to correctly answer questions about the carbon cycle.

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When retrieving the column-averaged dry-air mole fraction of carbon dioxide, or X_{CO_2} , from space-based instruments, one of the primary issues is the presence of clouds and aerosols. These contaminants can introduce large errors into a retrieval because they tend to modify the light path in ways that are difficult to quantify. In order to accurately measure the number of molecules of CO_2 in the column of air, the length of the light path must be known. If clouds and aerosols are present they can scatter the reflected sunlight in multiple directions, which can drastically alter the length of the light path seen by the sensor and result in significant errors when calculating X_{CO_2} . Neglecting scattering when measuring scenes containing clouds and aerosols can lead to substantial errors in X_{CO_2} . These errors are often in excess of 1% (~ 4 ppm of CO_2) and can be tens of ppm for scenes with thick cloud or aerosol layers (O'Brien and Rayner, 2002; Aben et al., 2007; Butz et al., 2009).

A common method used to avoid these large X_{CO_2} errors caused by light path modification is to parameterize clouds and aerosols explicitly within the X_{CO_2} retrieval. This often includes adding one or more scattering particle types to the retrieval along with variables that describe their optical and/or physical properties (e.g. optical depth, height of scattering layer, single scatter albedo) (Butz et al., 2009; Yokota et al., 2009; Crisp et al., 2010; Reuter et al., 2013; Parker et al., 2011). These particle types and corresponding properties are intended to represent typical clouds and aerosols found in the atmosphere. However, adding cloud and aerosol parameters to the retrieval algorithm can result in new issues such as creating an under-constrained problem or inducing nonlinearity in the forward model (Nelson, 2015). Further, it has been shown that these “full-physics” retrievals may incur biases from attempting to account for clouds and aerosols when none are present (O'Dell et al., 2012). For ideal, extremely clear scenes, this becomes an issue because the addition of a cloud and aerosol parameterization may be detrimental rather than beneficial. Additionally, a comparison of retrieved full-physics optical depths from build 3.4 (B3.4) of the NASA Atmospheric CO_2 Observations from Space (ACOS) X_{CO_2} retrieval algorithm (O'Dell et al., 2012; Crisp et al., 2010) to optical depths measured from the highly accurate AEROSOL ROBOTIC

NETwork (AERONET; Holben et al., 1998), shown in Fig. 1, revealed that the aerosol optical depths retrieved by the full-physics retrieval were not well correlated with the AERONET measurement for a particular scene.

The aforementioned problems associated with the full-physics retrieval algorithm motivated a study of a simplified non-scattering, or “clear-sky”, retrieval to test the hypotheses that it could provide comparably accurate X_{CO_2} measurements, given appropriate filtering of scenes contaminated by clouds and aerosols. These clear-sky retrievals are simple and highly linear because they assume no scattering or absorption effects caused by clouds or aerosols. Thus, clear-sky retrievals may avoid introducing unwanted biases when clouds and aerosols are not present. Recent work by Butz et al. (2013) has demonstrated that, for simulated measurements over ocean, a clear-sky retrieval can theoretically be used when scenes containing significant light path perturbations are removed. Correspondingly, this approach is now used in the operational RemoTeC retrieval (Guerlet et al., 2013; Butz et al., 2009).

Clear-sky retrievals are also desirable because of their high computational efficiency relative to full-physics retrievals. This is primarily because of the computational expense associated with calculating scattering from clouds and aerosols. The current operational ACOS algorithm takes roughly 10 min per measurement and OCO-2 collects about 10^6 measurements per day. This restricts the number of measurements able to be fully processed. The use of a clear-sky retrieval would thus, with current computational limits, allow for approximately one to two orders of magnitude more data to be processed. Additionally, the use of clear-sky retrievals would make it possible to perform repeated tests on large sets of data in significantly less time than if full-physics retrievals were used.

We begin by testing our hypothesis on simulated OCO-2 measurements then extend our analysis to real GOSAT measurements. We use various pre-filtering techniques to remove scenes obviously containing clouds and aerosols and employ the Data Ordering through Genetic Optimization (DOGO) system (Mandrake et al., 2013; Mandrake, 2015) to filter out additional contaminated measurements and improve the quality of

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4.3 DOGO: Data Ordering through Genetic Optimization

While the pre-filtering techniques we employed are effective at removing many scenes containing clouds and aerosols, other tools are needed to identify very clear scenes that are nearly free of cloud and aerosol contamination on which we believe X_{CO_2} retrievals will be most accurate. One method used to filter ACOS B3.4 data was a suite of approximately 18 tests to identify scenes of the highest quality, which tend to be the most clear (Osterman et al., 2013). In this study, the same genetic algorithm used to create OCO-2 Warn Levels (Mandrake et al., 2013; Mandrake, 2015) was employed to find optimal post-filters for both simulated OCO-2 and real GOSAT data. Unpublished studies have shown that this approach yields similar results to the 18-parameter hand-tuned filter, but with far fewer filtering parameters necessary. Additionally, while the hand-tuned procedure requires trial and error to find the best possible filters, DOGO is automated and can quickly find an optimum filter set with minimal hand-tuning required. For this work, DOGO attempted to find variables that, when used to filter a dataset, minimized the root-mean-square (RMS) of the X_{CO_2} error, where the X_{CO_2} error is defined as the difference between the retrieved X_{CO_2} and the true X_{CO_2} (described in Sect. 4.1). We chose this parameter because it instructs DOGO to remove outliers as well as reduce the overall bias, as the formula for RMS error includes both variance and bias. We also investigated applying a custom bias correction to the data prior to determining an optimal filter set, but found similar results. The parameters allowed for selection were all derived from the near-infrared measurements themselves, e.g. band signal levels, signal to noise ratios, retrieved surface pressure. The algorithm was not allowed to select certain variables, such as the validation X_{CO_2} or CALIPSO measurements (used to create the OCO-2 simulations). This was to ensure that DOGO did not “cheat” by having access to external information. Filtering was done for different “throughputs”, which equal the percent of data retained after filtering. The DOGO system can also use more than one “rule”, or filtering variable, when determining an optimal filtering strategy. That is, one rule selects the single most effective parameter at minimizing the X_{CO_2} RMS er-

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ror while two rules selects the best combination of two parameters in reducing the error. A larger number of rules results in a greater reduction in error for a given throughput, but typically only two to five rules are needed to maximize this reduction (Mandrake et al., 2013). In this study we used four rules and found that increasing the number of rules did not further reduce errors. DOGO was run separately for both clear-sky and full-physics retrievals as well as for land and ocean surfaces because it was hypothesized that different filtering parameters might be selected for each retrieval and surface type combination.

5 X_{CO_2} retrieval comparison

In the previous section we described our use of pre-filtering with the ABP and IDP and post-filtering with DOGO to produce a dataset with biases and outliers minimized to the greatest extent possible. Here we apply and evaluate our technique and examine the performance of the clear-sky X_{CO_2} retrieval compared to the full-physics X_{CO_2} retrieval for simulated OCO-2 and real GOSAT data. We evaluate the effectiveness of DOGO at reducing RMS errors, investigate the impact of cloud and aerosol optical depths on the OCO-2 simulations, and examine regional biases in the datasets by binning retrievals into the standard Atmospheric Tracer Transport Model Intercomparison Project-3 (TransCom-3) regions (Gurney et al., 2003).

5.1 Summary of OCO-2 error statistics

We begin by evaluating the performance of the clear-sky retrieval on OCO-2 simulations. Figure 4 demonstrates the effectiveness of DOGO at reducing X_{CO_2} RMS errors as a function of throughput. The initial reduction in error at high throughputs is dramatic, as the algorithm is easily able to identify and remove highly contaminated scenes. All datasets begin to plateau at approximately 50–80 % throughput as DOGO has already removed the obviously contaminated scenes and is now selecting the best of what re-

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aerosol layers as well as their interaction with the surface. However, the X_{CO_2} RMS errors become more comparable at lower throughputs, with the clear-sky retrieval error coming within a tenth of a ppm of the full-physics retrieval error at a throughput of 30 %. This is consistent with our hypothesis that when scenes contaminated by clouds or aerosols are removed, the clear-sky retrieval can perform as well as the full-physics retrieval. However, to demonstrate this explicitly, we must show that DOGO is indeed filtering out those scenes containing appreciable amounts of clouds and aerosols.

Because we know the true profiles of clouds and aerosols used to create these simulated OCO-2 measurements, this is straightforward. Figure 5 shows the binned X_{CO_2} RMS error vs. the true total optical depth (the sum of the true aerosol, ice cloud, and water cloud optical depths from CALIPSO, used to create the synthetic measurements) for clear-sky retrievals (left panel) and full-physics retrievals (right panel) over ocean. Yellow corresponds to 100 % throughput, green to 80 % throughput, and blue to 30 % throughput. At 100 % throughput, there are a significant number of thick ($\tau > 1.0$) cloud or aerosol scenes present, along with a secondary peak of thinner cloud or aerosol scenes. These thick scenes are primarily water clouds near the surface that the ABP was unable to identify and remove. In general, the 100, 80, and 30 % throughput X_{CO_2} RMS errors for clear-sky and full-physics retrievals over ocean are nearly equivalent, which agrees with our analysis of the ocean retrievals plotted in Fig. 4. For high optical depth scenes at 100 % throughput, the RMS error of the data is large (over 8 ppm for both retrieval types). This indicates that, as hypothesized, both retrieval types have large errors for scenes containing thick cloud or aerosol layers. Going from 100 % throughput (yellow) to 80 % throughput (green), DOGO greatly reduces the number of these high optical depth scenes, which corresponds to the steep initial decline of the ocean retrieval RMS errors in Fig. 4. This is impressive because, as was explained in Sect. 4.3, DOGO is not allowed to use the true optical depth as a filter, indicating that it is using other parameters to infer the amount of clouds and aerosols in a given scene. For example, the IDP filters are often selected by DOGO, which indicates that they are functioning as anticipated and properly identifying scenes containing clouds

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and aerosols. At 80% throughput, the full-physics retrieval has slightly smaller RMS errors than the clear-sky retrieval for scenes containing a moderate amount of clouds or aerosols ($0.1 < \tau < 1.0$). This supports our hypothesis that the full-physics retrieval's parameterization of clouds and aerosols is helpful for these types of scenes and that the clear-sky retrieval struggles because it is unable to account for the light path modifications caused by these contaminants. When only 30% of the ocean data remains (blue histogram), primarily low optical depth scenes ($\tau < 0.3$) remain and the clear-sky retrieval performs about as well as the full-physics retrieval in terms of both precision and bias, as the RMS errors are nearly identical. Additionally, the precision and bias were analyzed separately (not shown) and found to be similar. One might think that even slightly contaminated scenes ($\tau \sim 0.1\text{--}0.3$) should have been removed for the 30% throughput case, but DOGO's goal is to minimize the X_{CO_2} RMS error, not simply to remove scenes with high optical depths.

A similar analysis was performed for land scenes, with the results displayed in Fig. 6. As was seen over ocean in Fig. 5, at larger throughputs, higher optical depths correspond to larger RMS errors in the X_{CO_2} data. The clear-sky retrieval struggles with these high optical depth scenes, but also has relatively large RMS errors (~ 3 ppm) for moderate to small optical depths. As the throughput decreases, the RMS error becomes smaller and more uniform over the entire range of optical depths for both retrieval types. Interestingly, at a throughput of 30% some high optical depth scenes ($\tau > 1.0$) for the clear-sky retrieval over land still remain. However, the RMS error is still optimally reduced by DOGO and only $\sim 10\%$ worse than the full-physics retrieval. For the full-physics dataset, DOGO chooses to remove nearly all of these thick cloud or aerosol scenes. This suggests that the clear-sky retrieval is less sensitive to some high optical depth scenes over land, perhaps due to complex light path cancellation effects.

In addition to the statistical analysis of the full dataset, spatial errors in the OCO-2 retrieval datasets were analyzed to see if regional variability existed and if there were regions where the clear-sky retrieval had relatively small errors compared to the full-physics retrieval. These regional X_{CO_2} RMS errors for the simulated OCO-2 datasets

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ever, even at low throughputs (less than 60 %), the clear-sky retrieval dataset still has RMS errors roughly 30–60 % larger than those of the full-physics retrieval. This is in contrast to our simulation-based OCO-2 results, suggesting that additional unknown real-world mechanisms not included in the simulations may limit the ability of the clear-sky retrieval on real measurements over ocean surfaces. It is also possible that, despite promising results from our simulation-based tests, our filtering technique is unable to sufficiently remove scenes contaminated by clouds and aerosols over ocean surfaces. Another striking feature in this result is how effective the full-physics retrieval performs over ocean, even for highly contaminated scenes. At 100 % throughput, it still has RMS errors less than 2 ppm, implying that the more homogeneous nature of the ocean surface allows for the full-physics algorithm to successfully capture the influence of cloud and aerosol scattering effects.

Over land, the clear-sky retrieval (dashed orange line) has errors similar to the full-physics retrieval (solid orange line) when only modestly filtered by DOGO (throughput of ~ 80 %), which qualitatively reproduces our simulation-based results. The slopes of the initial decreases in RMS error over land are steeper than those for ocean. This may suggest that DOGO is more effective at initially removing contaminated or low quality measurements over land surfaces, despite having access to and using similar filtering variables. This may be due to photons scattering multiple times between cloud or aerosol layers and the surface and producing a more distinguishable signal for DOGO to filter on than for ocean surfaces, where photons are much less likely to scatter off the surface multiple times (due to glint angle geometry).

The X_{CO_2} RMS errors for the TransCom regions are shown in Fig. 9. The left panel shows the RMS error for the GOSAT full-physics retrieval dataset while the right panel shows the same but for the GOSAT clear-sky dataset. The datasets shown were post-filtered using DOGO with a throughput of 30 %. Over ocean, the clear-sky retrievals (right) consistently have regional X_{CO_2} RMS errors 40–60 % larger than the full-physics retrievals (left). The results over land surfaces are more variable. While the global mean difference in RMS error over land at 30 % throughput is 0.1 ppm, or ~ 10 %, this differ-

ence, when regionally analyzed, can be positive or negative. Certain regions, such as Northern Africa, have lower full-physics retrieval RMS errors but others, such as South America, have slightly lower clear-sky retrieval RMS errors. This regional variability could be due to heterogeneous surface characteristics or cloud and aerosol compositions compared to the relatively uniform ocean. Thus, we can not say with confidence that clear-sky retrievals perform better or worse over land surfaces for real GOSAT data without further investigation, but in general the two retrievals are surprisingly equivalent over land.

6 Conclusions

In this study we evaluated the performance of non-scattering, or “clear-sky”, X_{CO_2} retrievals from hyperspectral near-infrared measurements of reflected sunlight by comparing them to “full-physics” X_{CO_2} retrievals, which include scattering by clouds and aerosols. From our statistical analysis, we conclude that clear-sky X_{CO_2} retrievals typically do not perform as well as full-physics X_{CO_2} retrievals when no filtering is applied, consistent with previous findings. However, with the application of pre- and post-filters to remove low quality measurements contaminated by clouds and aerosols using only information contained in the near-infrared measurements themselves, our OCO-2 simulation-based tests demonstrate that clear-sky retrievals are of similar or only slightly reduced quality compared to the full-physics retrieval, depending on filtration level. This finding holds for real GOSAT observations over land, but not over ocean surfaces. For GOSAT measurements over land, the clear-sky retrieval has errors similar to those of the full-physics retrieval. For GOSAT measurements over ocean surfaces, the clear-sky retrieval has X_{CO_2} RMS errors 30–60% larger than those of the full-physics retrieval when the datasets are modestly filtered. The source of this extra error in the clear-sky retrieval applied to real GOSAT ocean measurements is unclear at this point and requires further study. Analysis of real OCO-2 measurements, which were unavailable during the time of this work, may help answer this question.

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For OCO-2 simulations and real GOSAT measurements over both land and ocean surfaces, the clear-sky retrieval has X_{CO_2} RMS errors less than 2.0 ppm when the dataset is sufficiently filtered. In addition, clear-sky retrievals can be one to two orders of magnitude faster than full-physics retrievals, as scattering by clouds and aerosols can be completely ignored. For sensors that collect enormous volumes of data, such as OCO-2, this could allow for significantly more data to be processed. Thus, clear-sky X_{CO_2} retrievals may be useful for certain applications that require a larger number of retrievals but have less stringent error requirements. Further, estimates of parameters, such as surface albedo, from a clear-sky retrieval could serve as a useful first-guess for the full-physics retrieval. The faster processing and more accurate first-guess values could be of even greater utility to future satellite missions that will likely make even more measurements than OCO-2.

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Table 1. Properties of the full-physics and clear-sky X_{CO_2} retrievals.

Type	Bands Used (μm)	Clouds & Aerosols Parameterized	P_{stc}	Source
Full-Physics	0.76, 1.6, 2.0	Yes		O ₂ A-band
Clear-Sky	1.6, 2.0	No		ECMWF

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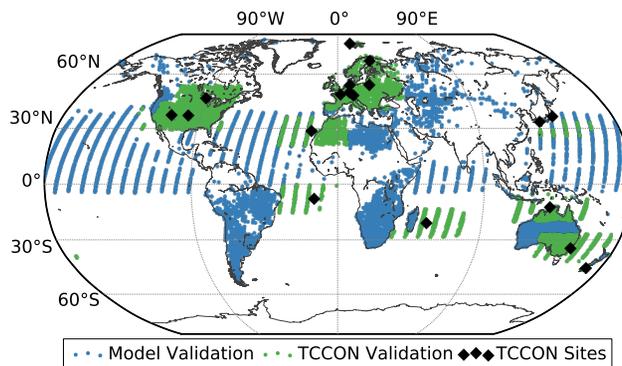


Figure 2. Global distribution and X_{CO_2} validation source of the 25 000 GOSAT measurements.

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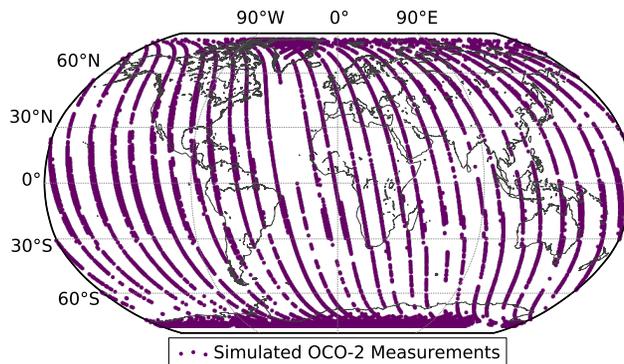


Figure 3. Global distribution of the 44 000 simulated OCO-2 measurements.

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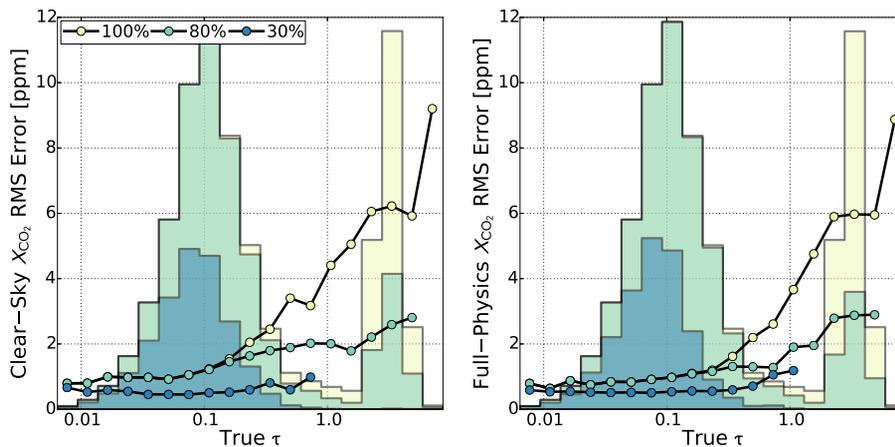


Figure 5. Clear-sky (left) and full-physics (right) X_{CO_2} retrieval RMS errors vs. the true total optical depth for simulated OCO-2 measurements over ocean. The black lines are binned averages of the X_{CO_2} RMS error for 100 % throughput (yellow markers), 80 % throughput (green markers), and 30 % throughput (blue markers). The histograms represent the relative amount of data for each throughput.

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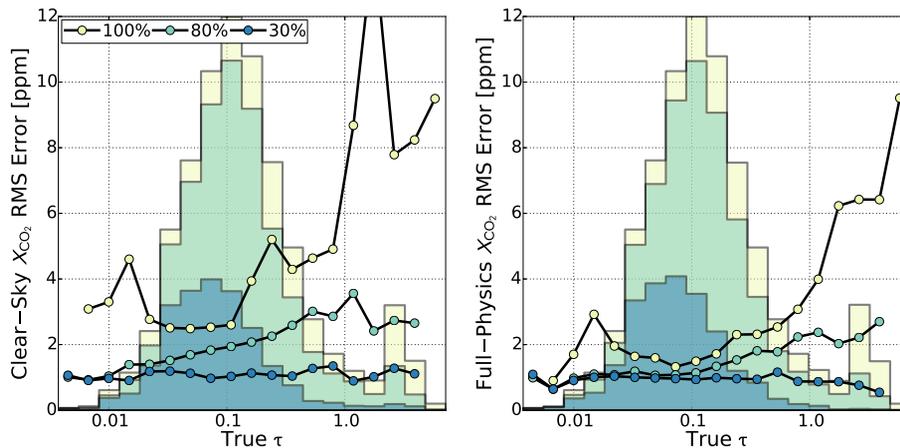


Figure 6. Clear-sky (left) and full-physics (right) X_{CO_2} retrieval RMS errors vs. the true total optical depth for simulated OCO-2 measurements over land. The black lines are binned averages of the X_{CO_2} RMS error for 100% throughput (yellow markers), 80% throughput (green markers), and 30% throughput (blue markers). The histograms represent the relative amount of data for each throughput.

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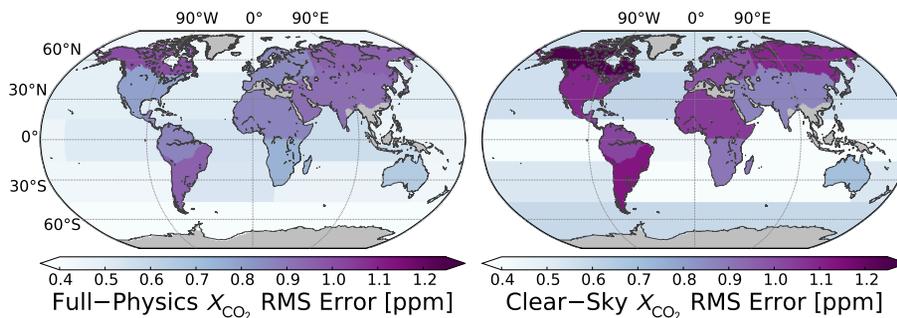


Figure 7. OCO-2 full-physics (left) and clear-sky (right) retrieval X_{CO_2} RMS errors for the TransCom regions with a throughput of 30 %.

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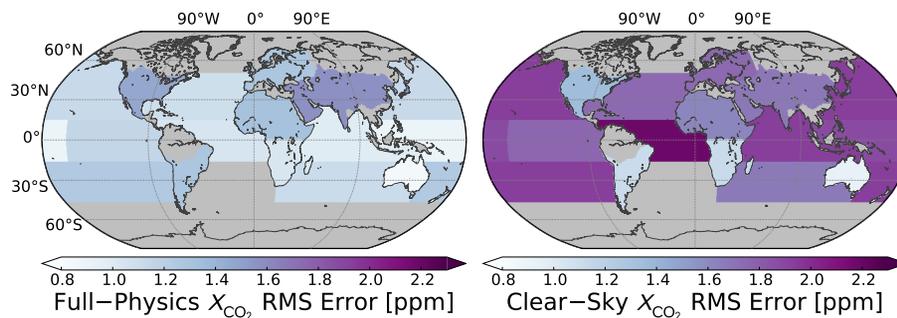


Figure 9. GOSAT ACOS B3.4 full-physics (left) and clear-sky (right) retrieval X_{CO_2} RMS errors for the TransCom regions with a throughput of 30 %.

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