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2016

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Schepers, D. (2016). *Observing atmospheric methane from space*. [PhD-Thesis – Research external, graduation internal, Vrije Universiteit Amsterdam].

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Conclusions

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The overall research presented in this thesis comprises an effort to thoroughly understand and improve methane total column retrievals from GOSAT short-wavelength infrared Earth-radiance observations. The first part of this thesis focussed specifically on characterising the performance of the proxy and physics-based retrieval schemes, focusing on their ability to accurately account for scattering of light in the Earth's atmosphere. To that end, a comparison and validation study was set up that revolved around the following research question:

> **Research question 1.** What is the difference between the proxy and physics-based retrieval methods concerning their ability to account for light path modification in total column methane retrievals from cloud-free GOSAT SWIR observations over land?

Within this study, total column methane abundances retrieved with both methods were compared and validated using methane total column measurements provided by 12 stations of the ground-based TCCON network as reference. Based on a 19-month data set of GOSAT soundings that are collocated with the 12 TCCON measurements sites, it was found that there is no significant difference in the performance of both retrieval strategies. Both methods show typical retrieval uncertainties that are well within one percent of the total column methane abundance. When compared on a global data set however, larger differences between the proxy and physics-based approaches became evident. A subsequent comparison of retrieved CH_4 abundances with assimilated methane fields from a global chemistry-transport model identified typical weaknesses in both retrieval approaches. These weaknesses can result in retrieval biases of up to 1% of $X_{\mathrm{CH_4}}$ on regional scales.

In case of the physics-based retrieval method, the total column CH_4 abundances are overestimated in regions where extensive atmospheric scattering exists over a highly reflective surface. These conditions are primarily found in the desert regions of North Africa and the Middle East. Retrieval errors in the proxy method are predominantly caused by inaccuracies in CO_2 abundances from a priori data. When using the proxy method, these inaccuracies propagate directly into the retrieved methane total columns. In this study, the latter manifested itself as an overestimation of the seasonal cycle amplitude over the Indian subcontinent, especially overestimating CH_4 mixing ratios in spring.

In light of these results, it is clear that the subset of GOSAT retrievals that are collocated with TCCON measurement sites are not representative for retrieval performance in other geographical areas. This effect was traced back to a limited range of typical surface albedos and aerosol loads around the TCCON measurement sites. This causes scattering conditions and light path effects to be very similar among different TCCON measurement sites, effectively limiting the validation study to only a subset of possible light path modification scenarios. Clearly, this is not an ideal situation for validating satellite-borne trace gas retrievals from SWIR, where atmospheric scattering forms a major source of uncertainty and properly accounting for light path modification constitutes the major challenge. Therefore, it is recommended that the TCCON network be extended to cover different geographical regions and a broader range of surface albedos. Since the publication of the foregoing results, the TCCON network has indeed been extended (e.g. TCCON Website).

Although the physics-based method showed reduced performance in cases of strong atmospheric scattering, it is least affected by uncertainties a priori data and has most potential for further development and improvement. Therefore, the remainder of this work focuses on further development of the physics-based retrieval, with the aim of making it more capable of processing soundings with enhanced scattering by aerosol and water clouds. As a first step, a new radiative transfer model was developed to reduce the numerical effort involved with forward model calculations under conditions of strong scattering:

> **Research question 2.** How to efficiently simulate the pronounced scattering of short-wavelength infrared radiation in a cloudy atmosphere and thereby enable physics-based methane retrievals from cloudy GOSAT observations?

The developed radiative transfer model, LINTRAN v2.0, is capable of modelling cloud contaminated satellite observations and their derivatives with respect to atmospheric and surface state variables in a numerically efficient manner. A significant gain in efficiency was achieved – with respect to its predecessor model – through a mathematical framework that combines an approximate iterative solving method with separation of the first N orders of scattering from the diffuse intensity vector field. Contributions to the observable up to order of scattering N are recursively solved in an analytical manner. Contributions from higher orders of scattering are subsequently solved in a numerical manner, assuming that the intensity field varies linearly with the vertical coordinate within an optically homogeneous model layer.

This method is implemented in LINTRAN v2.0, choosing $N = 2$, within the general framework of forward-adjoint perturbation theory. In cloudy atmospheres, the numerical performance of this radiative transfer model is significantly better than the previous model version, translating into speed-up of calculations with a factor 42 without a loss in model accuracy.

LINTRAN v2.0 was subsequently implemented in the forward model of the RemoTeC physics-based retrieval method. This algorithm is extensively used to retrieve CH_4 and CO_2 columns from GOSAT SWIR measurements over land. With LINTRAN v2.0 implemented in the forward model, the RemoTeC physics-based method was further developed for retrieving methane abundances form cloudy GOSAT soundings.

> **Research question 3.** In light of increasing data yield, can the physics-based retrieval method – using the newly developed radiative transfer model – be successfully applied to retrieve total column methane abundances from cloudy nadir observations?

This new version of the physic-based RemoTeC algorithm was subsequently applied to cloudy GOSAT nadir soundings over the ocean where a cloud layer is necessary to provide sufficient radiance signal over an otherwise non-reflective ocean surface. In this retrieval setup, all light scattering in the Earth's atmosphere is described by a single-layer water cloud with Gaussian height distribution. Together with the column abundances of CO_2 and CH_4, the height and the geometrical thickness of the cloud layer are inferred from the measurement as well as the cloud droplet size and their total amount.

The CH_4 and CO_2 column products were validated with ground-based total column measurements performed at 8 stations from the TCCON network that are geographically close to an ocean coastline. For the TCCON site with the most robust statistics, we find a retrieval bias of 6.14 ppb or 0.36% for X_{CH_4} combined with a standard deviation of retrieval errors of 18.89 ppb (1.15%). For X_{CO_2}, the bias is 1.96 ppm (0.51%) combined with a standard deviation of 4.00 ppm (1.03%). Averaged over all TCCON sites, our retrievals are biassed -5.87 ppb (-0.32%) for X_{CH_4} and -0.04 ppm (-0.01%) for X_{CO_2}. The standard deviation of station biases amounts to 6.23 ppb (0.35%) for X_{CH_4} and 1.77 ppm (0.45%) for X_{CO_2}.

In terms of retrieval accuracy and precision, the proposed physics-based methane retrieval for cloudy ocean soundings performs slightly worse than the RemoTeC physics-based method for cloud-free observations over land. However, being able to retrieve CH_4 from cloudy GOSAT soundings may significantly increase data coverage over the oceans where current GOSAT methane retrievals rely exclusively on observations in sun-glint geometry which severely limits their number and geographical coverage. Hence, methane retrievals over cloudy oceans do provide valuable extra information on methane abundances in areas that beforehand were only sparsely covered.

5.1 Outlook

By enabling physics-based methane retrievals from cloudy GOSAT soundings over the ocean, this work represents an important step toward increasing the applicability of the physics-based retrieval method. A natural follow-up would be to apply the proposed retrieval strategy to the complete (sub)set of cloudy GOSAT ocean observations, which would significantly increase geographical data coverage, especially in the Southern Hemisphere. Since retrievals in cloudy atmospheres lack sensitivity in the boundary layer, these retrievals will predominantly provide information on CH_4 in the free troposphere. In the context of global inversions of methane sources and sinks, this information is especially useful to constrain (long range) methane transport and the atmospheric methane sink. Furthermore, one might attempt similar retrievals from cloudy observations over land, targeting optically thick and unbroken cloud layers to minimise the effect of surface reflection, mimicking the situation over the non-reflective ocean surface.

Throughout this research, the importance of representative validation measurements has been apparent. In Chapter 2 it was shown that the network of ground-based validation sites available at the time was insufficient to identify key performance differences between the proxy and physics-based retrieval methods. In Chapter 4, the validation of satellite-born methane retrievals over ocean areas was based on a sparse set of island- and coastal measurement sites. Especially the latter cannot be considered fully representative of oceanic measurement conditions. It is thus essential that the set of ground-based total column measurements available for validation of such retrievals be extended to include a wide range of scenarios. This might be achieved by adding more permanent measurement sites or by adopting a more mobile measurement platform in combination with (dedicated) validation measurement campaigns. Considering this shortcoming in validation measurements, having two conceptually different retrieval methods – both with their own strengths and weaknesses –

proved valuable for identifying retrieval uncertainties in regions of the globe that are not directly covered by the validation network.

Acknowledgements

It has been about 5 years since I embarked on a path toward a Ph.D degree in the exciting field of satellite remote sensing. Today, this thesis marks the end of that journey. Back then, I could hardly have imagined what an interesting and enriching time it would be. Non of it would have been remotely possible without the support of so many people. Hence, I few heartfelt words of thanks are in order.

First and foremost, Jochen, I want to thank you for all your time and effort you put into this project as well as my M.Sc. project that came before. It was you after all who introduced me to the field of remote sensing of atmospheric trace gases –which at the time was quite alien to me– by agreeing to co-supervise my M.Sc. thesis. As evidenced by this thesis, your enthusiasm for the field proved to be contagious. Along the way, your willingness to share your expertise has been of great help while your general down-to-earth attitude often helped to put things into perspective. It was an absolute pleasure working together.

Ilse, I thank you for providing me with the opportunity to pursue this degree and for all your efforts that allowed me to obtain it.

It goes without saying that many more (former) colleagues at SRON's Earth division have, directly or indirectly, contributed to this work. You are all gratefully acknowledged! André, Haili, Otto, Rob and Sandrine, thank you all for the fruitful collaboration on developing the RemoTeC software and its application to GOSAT SWIR observations. Joost, I feel especially indebted to you for the great work you did on implementing the radiative transfer code. It would not have worked out so well without your efforts.

Also, I am grateful to all those colleagues that made SRON a particularly enjoyable place to work. Especially Andreas, Antonio, Arjen, Manuel, Pourya, Remco, Theodora, Tobias and the occasional Friday afternoon drinks frequenters. These afternoons, evenings, sometimes nights, were a thoroughly enjoyable –and effective– way to detach from work, to widen my knowledge and understanding on so many topics and to properly start the weekend.

Andreas and Theodora, it was an absolute blast sharing an office with you. Many, many long hours we've spent together sharing just as many frustrations, but after all, it was loads of fun all the way.

Finally, although not of least importance, I'd like to thank my parents, family and friends for their kind support and interest as well as for providing the necessary distractions from time to time. I'd like you to know that you've all added your indispensable contributions to this work.

Curriculum vitæ

Dinand Schepers was born in Hardenberg, The Netherlands on the 12th of May 1986. After completing his secondary education, he earned his B.Sc. degree in Aerospace Engineering from Delft University of Technology. He subsequently pursued a M.Sc. degree in Aerospace Engineering with a focus on Earth- and Planetary observation. In the course of this M.Sc. program, he undertook an academic internship at the GNSS Research Center of Wuhan University in the People's Republic of China. At the GNSS Research Center, he was involved in the reconstruction of precise orbits for the GRACE satellite tandem to assist studies of the Earth's gravity field being undertaken at Delft University.

For his M.Sc. graduation research, Dinand joined SRON The Netherlands Institute for Space Research. There he investigated the possibilities of using an artificial neural network to model satellite observations of solar light that is backscattered in the Earth's atmosphere in a fast and efficient manner. He subsequently accepted a Ph.D. position at SRON, working to improve the retrieval of atmospheric methane abundances from Earth-radiance measurements. This work, conducted between June 2010 and Dec 2014, ultimately resulted in this thesis.

In December 2014 Dinand joined S[&]T Corporation to contribute to the on-ground calibration campaign of the Sentinel-5 Precursor (TROPOMI) satellite instrument. In July 2015, after the successful end of TROPOMI on-ground calibration campaign, Dinand joined the research and development section at the European Centre for Medium-Range Weather Forecasts (ECMWF). There his work will be focussed on assimilation of a wide range of satellite observations in the context of multi-decadal reanalyses of the global climate system.

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