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Atmospheric Measurement Techniques Discussions

Exploring commercial GNSS RO products for Planetary Boundary Layer studies in the Arctic Region

Manisha Ganeshan[1,2], Dong L. Wu[1], Joseph Santanello[3], Jie Gong[1], Chi Ao[4], Panagiotis Vergados[4] and Kevin Nelson[4]

[1]Climate and Radiation Laboratory, NASA Goddard Space Flight Center, Greenbelt, 20771, USA
[2]Morgan State University, Baltimore, 21251, USA
[3]Hydrological Sciences Laboratory, NASA Goddard Space Flight Center, Greenbelt, 20771, USA
[4]NASA Jet Propulsion Laboratory, California Institute of Technology, Pasadena, 91109, USA

Correspondence to: Manisha Ganeshan (manisha.ganeshan@nasa.gov)

Abstract.

Commercial GNSS RO products are being touted for their coverage in polar regions where COSMIC-2 observations don't reach. This study seeks to explore their value for Arctic PBL investigations where sufficient lower atmospheric penetration of GNSS RO is vital for representing the persistently shallow PBL. Both NASA purchased commercial RO products, Spire and GeoOptics, have improved lower tropospheric penetration probability over the Arctic Ocean compared to MetOp observations, with Spire having greater volume of observations (nearly two orders of magnitude) compared to GeoOptics. A seasonal cycle is evident in the RO penetration probability (except for Spire) that is found to be related to the water vapor pressure. For winter months, at the 500m level, which is the standard cut-off threshold used for GNSS RO PBL studies, both products yield a penetration probability of ~80% of total observations over the Arctic Ocean and up to ~100% over the frozen sea ice region. As a result, both products are able to sufficiently represent the shallow Arctic PBLH (less than 300m depth) which is comparable to the PBLH from MERRA-2 reanalysis.

1 Introduction

The planetary boundary layer (PBL) is a target observable of broad importance to the Earth Science community and the Global Navigation Satellite System (GNSS) Radio Occultation (RO) is a candidate measurable approach for observing the PBL height (PBLH) as recommended by the National Academies of Science Decadal Survey for Earth Science and Applications from Space report (NASEM 2018, Teixeira et al. 2021). Today, advancing PBL science is inherently reliant on high resolution observations with high frequency sampling that can chiefly be afforded by a single remote sensing instrument/combination of instruments from space. In this regard, GNSS RO comprises a vital measurement technique due to its superior vertical resolution compared to most other space-based instrument technologies allowing penetration up to the lowest 100 meters above the surface. High vertical resolution measurements and deep penetration to the lower atmosphere

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are deemed vital for polar regions where it is particularly difficult to observe and characterize the persistent shallow PBL temperature inversion.

1.1 Importance of GNSS RO for Arctic PBL studies: Why commercial data?

The study of the Arctic Ocean PBL can greatly benefit from GNSS RO observations which offer (a) continuous sampling under all weather conditions, (b) the ability to "see" beneath the persistent stratus cloud cover, (c) improved predictability over flat surfaces (sea ice, open ocean) compared to varying slopes (land mass), and (d) long-term data record spanning nearly two decades with added coverage from recently launched commercial satellites. Commercial satellites are particular advantageous for high latitude polar studies where there is a notable lapse in coverage following the decommissioning of the Constellation Observing System for Meteorology Ionosphere and Climate (COSMIC-1) in 2018. The successor satellite, COSMIC-2, only covers 45°N to 45°S. It is expected that coverage from Spire and GeoOptics can help fill the gaps in the climate data record. First, however, it is necessary to explore the lower atmospheric sounding capability of these commercial missions in comparison to past and current existing operational GNSS RO products in the Arctic. Especially in the Arctic, the refractivity-based method used for determining the PBL height is found to be sensitive to the penetration capability of RO profiles (Ganeshan and Wu 2015). For example, from the analysis of 8 years of COSMIC data it was found that RO profiles over the Arctic Ocean dropped sharply at tangent heights below 1km, which introduces a sensitivity of the retrieved PBL height to the choice of the cut-off altitude used for profile selection. Therefore, it is worthwhile comparing the lower atmospheric penetration capability among various GNSS RO products and exploring factors that can influence this capability.

1.2 A background of GNSS RO neutral atmosphere technique

In the GNSS RO technique, the neutral atmosphere is considered as the atmospheric path consisting of the troposphere and stratosphere (up to 60km) which is refractive and electrically neutral, unlike the ionosphere. The neutral atmosphere has both dry and wet components that contribute to the refraction, with the wet component becoming more important closer to the surface. Not all RO profiles reach the surface, and in fact, there can be an exponential drop in the fraction of available RO observations (penetration probability) as we go towards the surface (Ganeshan and Wu 2015) which is primarily due to decrease in SNR caused by atmospheric defocusing effects (Wu et al. 2022). However, factors such as instrument design, neutral atmosphere excess phase computation method, and choice of bending angle processing algorithm can also affect the penetration probability profile for a given atmospheric path.

A thorough understanding of factors affecting RO penetration is desirable to help minimize sampling bias as well as to ensure data continuity and consistency in climate records. However, this is difficult to achieve, given the existence of vast number of GNSS RO missions and different versions of products from a single mission that are periodically reprocessed to remain up-to-date with advances in software and processing algorithms. This study aims to provide a comparison of the

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penetration capability of the new commercial and other existing GNSS RO data products in the Arctic as the first step towards establishing a climate ready, long-term continuous dataset that can be used for Arctic PBL investigations.

2 Datasets and Methodology

2.1 GNSS RO

2.1.1. Commercial datasets

The goal of this study is to explore the value of commercial GNSS RO products for PBL studies in the Arctic Ocean (north of 60°N excluding land areas) by comparing with other contemporaneous GNSS RO mission products such as COSMIC and the Meteorological Operational satellite programme (MetOp). The commercial GNSS RO data evaluated in this study are purchased by NASA through the Commercial SmallSat Data Acquisition (CSDA) program. In addition, this study also compares freely available commercial data purchased for near-real time operations by NOAA, for available brief periods of overlap with the NASA purchased commercial data.

NASA Spire data are available from Nov 2019 through Jan 2022, and NASA GeoOptics data are available from Jan 2020 to Apr 2021. Spire data are provided at a similar vertical grid and resolution as other GNSS RO missions (such as COSMIC, COSMIC-2, MetOp) where the lowest level of valid observations differs from profile to profile because the penetration depth achieved by each radio occultation is unique, depending primarily on the signal-to-noise ratio (SNR) profile. GeoOptics data, on the other hand, are provided on a uniform 100m vertical spacing grid, along with a quality flag that is used to determine the lowest penetration level. The quality flag is applied in two ways: (i) blanket criteria that checks the range of the amplitude of computed phase match integral and cumulative number of phase jumps within the upper neutral atmosphere (between 8 to 40 km), cutting off the profile at lower levels if the above checks are failed, and (ii) individual criteria that flags each level as "good" or "bad" based on the presence or absence of sharp features (moisture and temperature gradients) that can cause significant deviation of the bending angle relative to a smoothed background bending angle profile. In this study, only profiles satisfying the blanket criteria are considered as we are only evaluating the lower troposphere (surface to 5km), and moreover, profiles that pass the blanket criteria are evaluated individually to determine the minimum penetration depth ascertained by the lowest level with a "good" quality flag, thus automatically discarding atmospheric levels that occur below "sharp" atmospheric features.

The NOAA Spire and GeoOptics data purchased for near-real time operations are downloaded from the University Corporation for Atmospheric Research (UCAR; http://www.cosmic.ucar.edu/) website. In the case of GeoOptics, the overlap between NOAA and NASA data is during the month of April 2021, and for Spire, the month of October 2021 is chosen to compare overlapping data.

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2.1.2. Other datasets

In addition to NOAA commercial data, we also use COSMIC data and MetOp data from UCAR for comparisons with NASA purchased Spire and GeoOptics products. Two versions of reprocessed COSMIC data (COSMIC 2013 and COSMIC 2021) are obtained for the period ranging from 2007 to 2013 and from 2007 to 2017, respectively. Similarly, the post-processed MetOp data (metopa, metopb, and metopc) are also obtained from the UCAR website from Oct 2019 to Dec 2020. The MetOp data are available contemporaneously as the NASA commercial RO data, however, COSMIC data ceased to be produced at the time of launch of commercial satellites thereby limiting their use for comparative analysis.

2.1.3. Deriving PBLH from GNSS RO

The PBLH is derived from the GNSS RO refractivity profile using the bottom-up approach described in Ganeshan and Wu (2015), identifying the first minima of the refractivity gradient to exceed -40 N-unit km^{-1} and assigning the corresponding altitude as the PBLH. This approach is specifically useful for deriving the height of the PBL inversion over the Arctic during winter months. A cut-off altitude threshold, set to 500m, is applied to only include RO profiles that reach this altitude or lower. This is the typical cut-off altitude used for GNSS RO based PBL studies (Ao et al. 2012, Guo et al. 2011) that has also proven useful for Arctic PBLH retrieval (Ganeshan and Wu 2015).

2.2 Ship campaign observations

Recently, year-long radiosonde launches were performed over the frozen Arctic Ocean as part of the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) expedition that involved taking measurements from a transpolar drifting ice-breaker, R/V Polarstern, from Oct 2019 to Sep 2020. During MOSAiC, radiosondes were launched at least every 6 hours for the duration of the expedition (Männel et al. 2021). Using the temperature in the radiosonde dataset (Maturilli et al., 2021) and applying the World Meteorological Organization (Jarraud 2008) equation (eq. 1), one can estimate the saturation vapor pressure at each level. In the following equation, e_w is the saturation vapor pressure in hPa, and t is the temperature in K.

$$e_w = 6.112\, e^{(17.62\, t/(243.12 + t))} \quad \text{(eq. 1)}$$

After deriving e_w, it is possible to infer the water vapor pressure (wvp) using the percentage relative humidity from radiosonde (RH) and applying eq. 2:

$$wvp = e_w * RH * 0.01 \quad \text{(eq. 2)}$$

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The average daily wvp and wvp gradients are calculated at different levels (500, 600, and 700m) in order to test the robustness of the relationship between moisture and RO penetration probability at various altitudes. The wvp gradient at a given altitude is simply the rate of change of wvp within a 100m layer at that altitude.

2.3 Reanalysis data

The MERRA-2 reanalysis product (Gelaro et al. 2017) is used to obtain monthly mean water vapor pressure, monthly mean sea ice cover and monthly mean PBL height over the Arctic Ocean. The horizontal resolution of MERRA-2 products are approximately ~0.5 degree, and the GNSS RO derived monthly mean penetration probability and monthly PBL height characteristics are interpolated on the MERRA-2 grid for ease of comparison. Note that the MERRA-2 water vapor is obtained at the 5th level on the model native grid, which approximately corresponds to ~500m altitude.

3 Results and Discussions

3.1 Coverage over Arctic Ocean

GNSS RO profiles of bending angle and refractivity observations are characterized by a loss of signal (decrease in SNR) as we approach the surface due to atmospheric defocusing effects (Wu et al. 2022). However, the rate of penetration loss is expectedly different for various RO missions due to diversity in the design of GNSS receivers and SNR capabilities, but it can also be different for measurements from the same instrument due to inherent disparity in excess phase computations and bending angle retrieval algorithms. For example, older versions of the same product, such as COSMIC 2013, can differ significantly from newer reprocessed versions (COSMIC 2021) due to advances in excess phase computations, retrieval software, GNSS orbits, clock, and earth orientation products (UCAR Data Release, 2022).

Figure 1 compares the rate of RO penetration loss over the Arctic Ocean for different GNSS RO missions (COSMIC, MetOp, Spire, GeoOptics) as well as for different products from the same mission (COSMIC 2013 vs. COSMIC 2021; Spire NASA vs. Spire NOAA; GeoOptics NASA vs. GeoOptics NOAA). Clearly, the penetration loss is less significant for the newer version of COSMIC data (COSMIC 2021) compared to older products (COSMIC 2013, MetOp) due to the aforementioned major advances in computations and retrieval software. For contemporaneously processed data products, such as Spire NASA vs Spire NOAA and/or GeoOptics NASA vs. GeoOptics NOAA, there are differences in penetration probability but these are generally confined to the lowest 1 km. Moreover, the fraction of observations reaching the lower atmosphere (up to 500 m) is generally improved for these products compared to COSMIC 2013 and MetOp data. Note that this improvement in penetration probability is perhaps unique for the Arctic region as this evaluation doesn't consider the tropics and other midlatitude regions where GeoOptics data appear to have poorer lower atmospheric penetration compared to COSMIC-2 (not shown).

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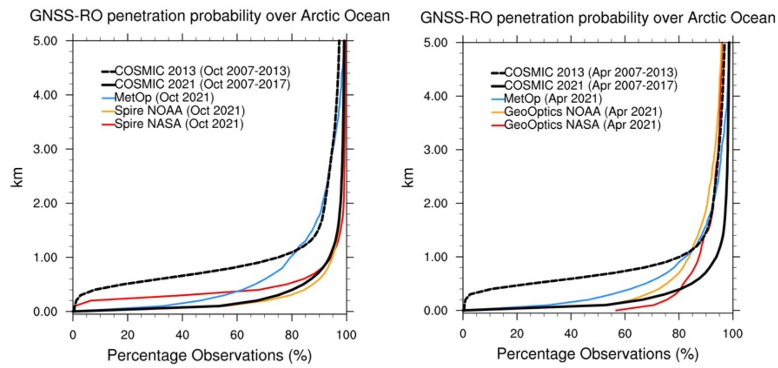

Fig. 1 The penetration probability of GNSS RO over the Arctic Ocean (north of 60°N) from different products comparing **(left)** COSMIC, MetOp, Spire for the month of October and **(right)** COSMIC, MetOp, GeoOptics for the month of April.

For most studies involving RO-derived PBLH, including the Arctic region, a 500m cut-off altitude is chosen to select profiles used for retrieving the PBLH, with the caveat that this threshold may not be ideal for representing shallow PBLs (Ao et al. 2012; Ganeshan and Wu 2015). Regardless, the 500m level is chosen in this study, and Figure 2 compares the time-series of penetration statistics among various RO products at this level. Even though the total number of observations are fewer for GeoOptics (by an order of magnitude compared to Spire data), the percentage of available observations is comparable between both products. In fact, during winter months over the Arctic Ocean, nearly 80% of commercial GNSS RO observations reach 500m, versus only ~65% for MetOp data which confirms that the RO sampling needed for Arctic PBL evaluation is much improved in commercial RO products.

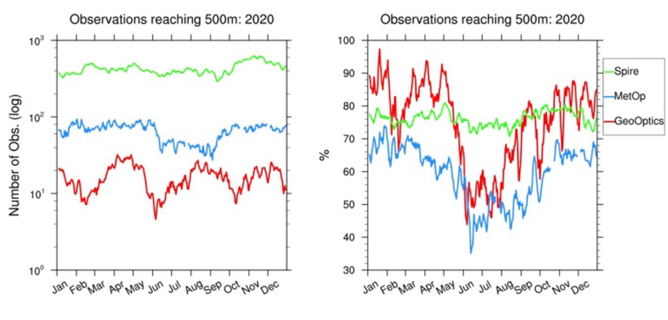

Fig. 2 Annual time-series of **(left)** number of observations and **(right)** percentage of total observations reaching 500m altitude or lower over the Arctic Ocean for the year 2020. The daily observations are smoothed using a 5-day running average filter. Note that contemporaneous COSMIC observations are not available for the purpose of valid comparison.

A seasonal cycle is evident in the penetration probability for GeoOptics and MetOp data with a minimum observed during summer months (right panel of Fig. 2). Such a seasonal cycle is consistently observed in the multi-year climatological

COSMIC data (not shown as contemporaneous observations are not available for comparison). The seasonality appears to be related to moisture. It has been previously speculated that the lack of penetration of COSMIC GNSS RO in the tropics is likely correlated with water vapor abundance (Ao et al. 2012, Chang et al. 2022) and the greater penetration over the ice-covered Arctic Ocean is due to the generally lower moisture content over the north pole (Ganeshan and Wu 2015). The following section will attempt to explore the relationship between penetration probability and water vapor using ship-based observations from the MOSAiC campaign. Note that the seasonal cycle is evidently missing in NASA Spire data (right panel of Fig. 2), although it is present in NOAA purchased Spire data (not shown).

3.2 Relationship between atmospheric moisture and GNSS RO penetration

As previously speculated (Ao et al. 2012, Ganeshan and Wu 2015, Chang et al. 2022), there is an apparent negative relationship between water vapor amount and RO penetration depth, with an increased capability for lower atmospheric penetration being typically observed in regions away from the tropics, including higher penetration values observed specifically over the dry north pole. In order to substantiate this with in-situ measurements, water vapor pressure (wvp) from radiosonde data as part of the MOSAiC campaign are used in conjunction with daily penetration probability measurements from MetOp data. During the MOSAiC campaign, radiosonde launches were made ~4 x daily from ice-breaker R/V Polarstern (Männel et al. 2021), allowing high vertical resolution sampling of the Arctic atmosphere throughout the year. Figure 3 shows the ship tracks for four months with each dot representing the location at the time of radiosonde launch. For most of the months, excluding the beginning and ending of the expedition, R/V Polarstern is anchored on a slow drifting ice-floe and the ship tracks are therefore confined to a limited latitude and longitude range. For each day, the mean daily location, average wvp, and average wvp gradient are estimated at three different levels (500m, 600m, and 700m) based on radiosonde launches. The RO penetration probability based on MetOp data is estimated around a 10° circle surrounding the daily ship location and at corresponding altitude levels. Figure 3(b) shows the time-series of the RO penetration probability and the water vapor pressure at 600 m level, and a strong negative correlation is indeed found to exist. The negative correlation similarly exists for other levels (500m and 700m) but it is strongest at this level. The correlation with wvp gradient and RO penetration probability is weaker (not shown). Thus, Figure 3 establishes that RO penetration probability and atmospheric moisture are indeed negatively correlated. This relationship is further explored by considering each month representing different seasons (Fig. 4), and is found to be strongest during the cold season (winter and spring) while being negligible during summer months and early fall (Jun-Sep).

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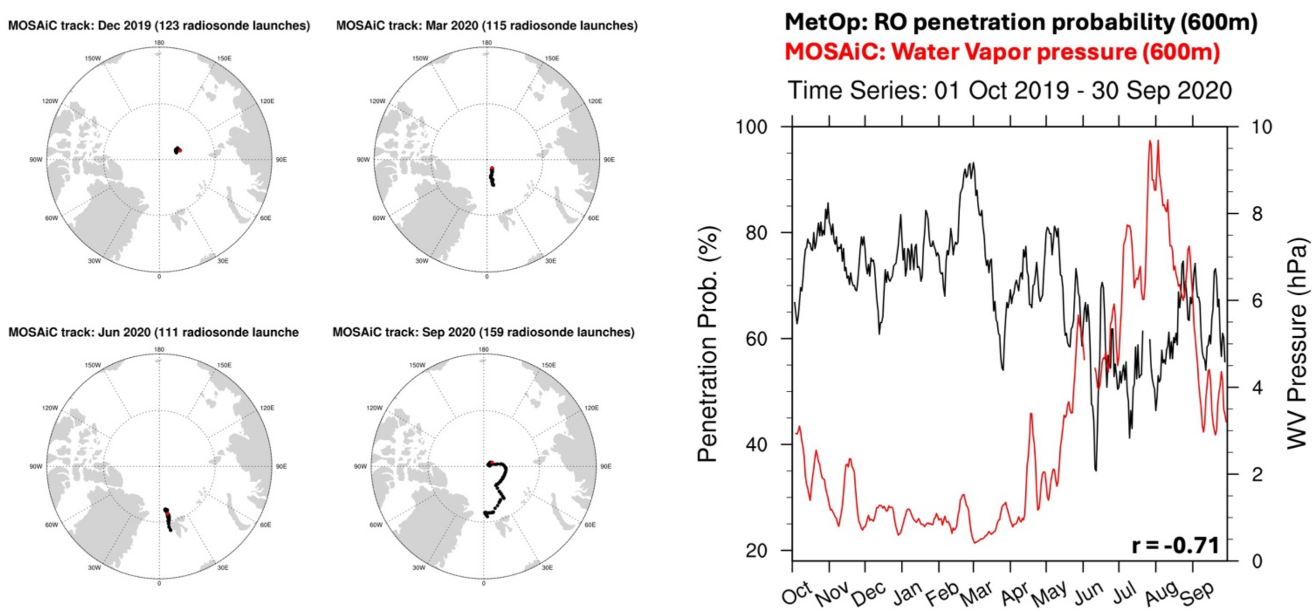

Fig. 3 (left) Examples of monthly ship tracks of R/V Polarstern during the MOSAiC expedition where each dot corresponds to the position of radiosonde launches (4xdaily) from the ice-breaker with the starting position indicated by the red dot, and **(right)** annual time-series of 5-day running mean of water vapor pressure from radiosonde (red) and corresponding RO penetration probability from MetOp (black) at 600m altitude obtained during the course of the MOSAiC expedition (from Oct 2019 – Sep 2020). The correlation coefficient *'r'* is indicated in the plot.

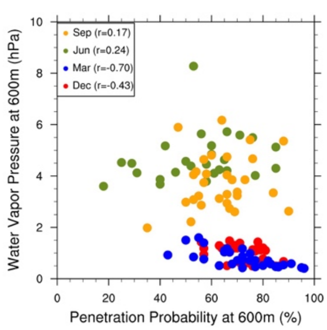

Fig. 4 Scatter plot showing the correlation between daily mean water vapor pressure from radiosonde and corresponding MetOp RO penetration probability at 600 m altitude for Dec 2019 (red), Mar 2020 (blue), Jun 2020 (green) and Sep 2020 (orange).

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3.3 Performance of commercial GNSS RO datasets for PBL retrievals over Arctic

This section will focus on exploring the potential for using commercial RO data for Arctic winter PBL studies using the cut-off altitude threshold of 500m to select RO profiles, as described previously (section 2.1.3 and section 3.1). Ganeshan and Wu (2015) showed that the minimum refractivity gradient method works well to detect PBL temperature inversions over the Arctic Ocean during winter months. Due to the lack of moisture in the atmosphere, the refractivity gradient minima is found to be sensitive to the positive temperature gradient maxima (i.e. temperature inversions).

Figures 5 (a-c) compares the 500m RO penetration probability for Dec 2020 obtained from MetOp, Spire, and GeoOptics data. In general, the penetration probability is higher away from coastlines due to the lack of influence of terrain elevation which was also noted in COSMIC observations (Ganeshan and Wu 2015). In addition, the penetration pattern agrees with previous studies that report a negative correlation with atmospheric moisture. Figures 5(d-g) suggests a generally good agreement spatially (negative correlation) with MERRA-2 water vapor indicating more penetration over drier sea ice regions compared to open ocean. This is consistent with COSMIC observations (Ganeshan and Wu 2015). The relationship between penetration probability and water vapor pressure is stronger for MetOp observations followed by GeoOptics, but is generally weaker for Spire data. The penetration probability of NASA purchased Spire data appears to be fairly independent of atmospheric water vapor distribution, a unique and slightly contradicting phenomenon compared to the penetration probability associated with other RO products that have strong empirical relationship with moisture (as observed in section 3.2). One commonality between the two commercial GNSS RO products is the increased penetration probability, particularly over the ice-covered region, where between 75-100% observations reach 500m altitude versus only 65-80% observations for the MetOp data.

Figure 6 compares the monthly RO-derived PBLH characteristics for each product. The adopted methodology (Ganeshan and Wu 2015) appears to work well for both commercial GNSS RO products, which clearly show the expected distribution of shallow PBLH over sea ice versus deeper PBLH over the Atlantic sector (left panel of Figs. 6 (a),(b)), with GeoOptics showing a stronger constrast between the two regions. On the other hand, Spire derived mean PBLH appears to have lesser regional and local variation compared to GeoOptics, as well as smaller standard deviation in derived PBLH (right panel of Figs. 6(a),(b)), which can be expected because of the increased vertical smoothing applied to their bending angle product (Bowler 2020) that may limit the effective vertical resolution of refractivity and the range of refractivity-derived PBLH values. Both commercial products show lower PBLH values over the sea ice compared to MetOp (right panel of Fig. 6(c)) and COSMIC (Ganeshan and Wu 2015), suggesting that the increased penetration probability (of up to ~100%) could play an important role in representing shallow PBLH in this region. Although a cut-off altitude of 500m has been regarded as sufficient for deriving refractivity-based PBLH from COSMIC RO observations in the past, it has been noted to be less than ideal for inferring PBL depth in the case of shallow PBLs (Ao et al. 2012) and may even contribute to a positive bias in regions such as the central Arctic Ocean (Ganeshan and Wu 2015). It appears, however, that the 500m cut-off altitude when applied to commercial GNSS RO products is sufficient for obtaining a realistic representation of the shallow Arctic PBLH. Note that a similar analysis was carried out for the GeoOptics data without imposing their recommended quality flag, and the resulting values of PBLH are found to be much higher suggesting that the vendor provided quality criteria are necessary for high latitude PBL studies.

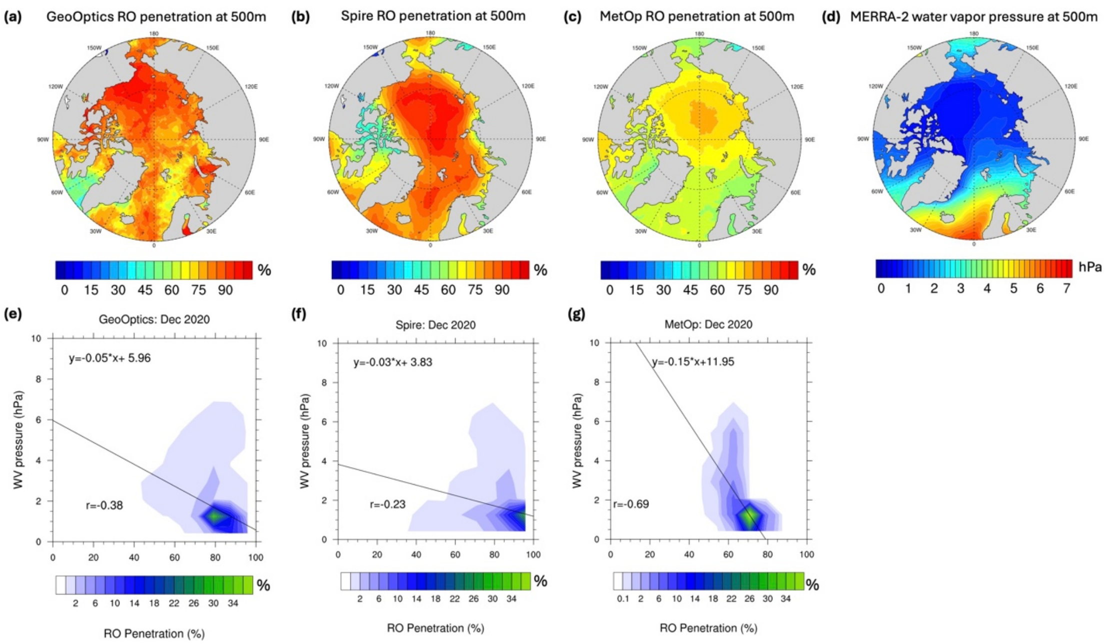

Fig. 5 (top) Arctic maps showing the monthly mean penetration probability of GNSS RO measurements reaching 500m altitude from **(a)** GeoOptics, **(b)** Spire, and **(c)** MetOp, and **(d)** the monthly mean water vapor pressure from MERRA-2 at approximately 500m altitude for Dec 2020, and **(bottom)** bivariate probability density functions of MERRA-2 water vapor at approximately 500m altitude and the 500m RO penetration probability for Dec 2020 from **(e)** GeoOptics, **(f)** Spire, and **(g)** MetOp data.

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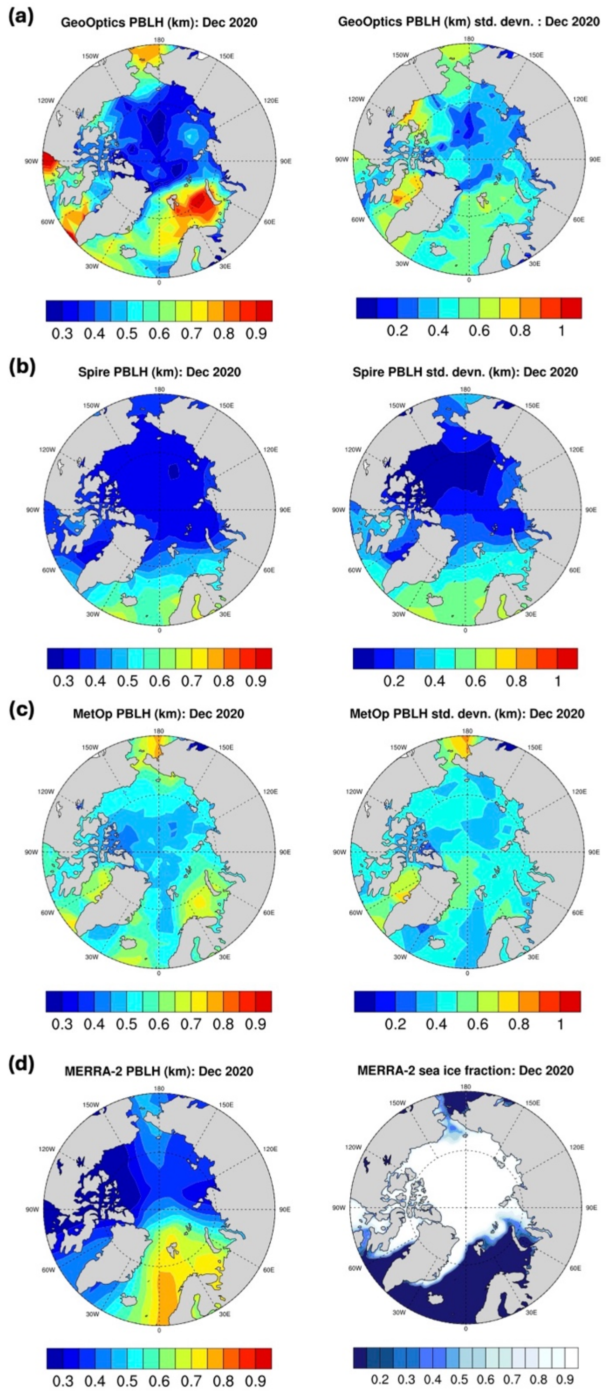

Fig. 6 Monthly PBL and surface characteristics for Dec 2020 showing **(left)** mean PBLH (km) derived from **(a)** GeoOptics, **(b)** Spire, **(c)** MetOp, and **(d)** MERRA-2 data and **(right)** standard deviation of PBLH (km) from **(a)** GeoOptics, **(b)** Spire, **(c)** MetOp, and **(d)** MERRA-2 fractional sea ice cover.

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4 Summary and Conclusions

This study explores the use of commercial GNSS RO neutral atmosphere products from Spire and Geoptics to advance Arctic PBL studies. The launch of commercial GNSS RO CubeSat receivers such as Spire and GeoOptics is especially opportune for high-latitude PBL studies which are presently recovering from the loss of COSMIC-1 and the lacking coverage by its successor COSMIC-2. In order to potentially advance PBL studies in polar regions, the new GNSS RO products must have sufficient lower atmospheric penetration capability, and the ability to sample shallow PBL temperature inversions that often persist in polar regions. This study attempts to provide a comparison of the penetration capability of the new commercial and other existing GNSS RO data products in the Arctic as the first step towards establishing a climate ready, long-term continuous dataset that can be used for Arctic PBL investigations.

Both commercial products, purchased by NASA, are found to have an improved lower atmospheric penetration capability over the Arctic Ocean compared to contemporaneous MetOp observations obtained from UCAR. The penetration capability is comparable to the newly reprocessed COSMIC data (COSMIC 2021). For an altitude of 500m or lower, the penetration probability from commercial RO products ranges from 75-100% for winter months over the ice-covered Arctic Ocean, which is significantly higher than MetOp (65-80%). The resulting PBLH derived from the commercial RO products is much lower over the ice-covered ocean (with values falling below 300 m in some regions) and in better agreement with MERRA-2 reanalyses data.

In addition, this study also uses an empirical approach to verify the previously speculated relationship between atmospheric moisture and RO penetration probability, using radiosonde observations from the recent MOSAiC expedition to derive atmospheric water vapor characteristics and MetOp observations to derive the corresponding penetration probability. It is found that there is indeed a negative correlation between atmospheric water vapor pressure (wvp) and penetration probability, which is evident mainly during the cold season months (Oct – May). The negative relationship between penetration probability and water vapor is also observed for other RO products, including GeoOptics, however, it is not clearly noticeable in NASA Spire observations.

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