

## **acpd-2017-640 Reply to Referee Comments**

### **Accuracy and precision of lower stratospheric polar reanalysis temperatures evaluated from A-train CALIOP and MLS, COSMIC GPS RO, and the equilibrium thermodynamics of supercooled ternary solutions and ice clouds**

**A. Lambert and M. L. Santee**

We thank the reviewers for their careful reading of the manuscript and appreciate their suggestions for improvements. We address their specific comments in the following text and outline the expected changes to the revised manuscript accordingly.

We have removed 3 of the 21 figures in the original manuscript (Figures 9, 14 and 15 in previous manuscript numbering).

The revised manuscript has 2 new figures (in response to referee comments) for a total of 20 figures (Figures 3 and 18 in revised manuscript numbering).

Referee Comments RC1/RC2 are in blue type.

Author Responses are in brown type.

## RC1 General Comments:

In this new paper Lambert and Santee evaluate lower stratospheric polar reanalysis temperatures by comparison with CALIOP, MLS, and COSMIC GPS measurements. In particular, the study focuses on the analysis of ice and STS equilibrium temperatures of PSC particles. Overall, I found this to be an interesting and carefully conducted study.

The paper is well-written, concise, and fits in the scope of ACP. I would recommend it for publication once the specific comments listed below have been addressed.

We will address the concerns of the referee in the modified manuscript. We reply to specific comments below.

## RC1 Specific Comments:

abstract: The abstract is a bit long and could possibly be shortened. At p2, l21-22 a copyright statement and acknowledgement was introduced, which seems to be out of place?

We agree that the abstract is a bit long and it has been shortened. Copyright and acknowledgement were placed following a request by the editorial support office.

p3, L13-15: At this point the reader might wonder why NAT is not considered in this study? The reason is given later in the manuscript (at the begin of Sect. 3), but I would like to suggest to move the explanation a bit forward.

A brief explanation was added.

p4, L6-10: Regarding the long-duration balloon observations there is a number of other studies using them for evaluation of meteorological reanalyses in the polar stratosphere (some of the papers being part of the recent S-RIP special issue in ACP):

Boccara et al., Accuracy of NCEP/NCAR reanalyses and ECMWF analyses in the lower stratosphere over Antarctica in 2005, *J. Geophys. Res.-Atmos.*, 113, D20115, doi:10.1029/2008jd010116, 2008.

Friedrich et al., A comparison of Loon balloon observations and stratospheric reanalysis products, *Atmos. Chem. Phys.*, 17, 855-866, <https://doi.org/10.5194/acp-17-855-2017>, 2017.

Hoffmann et al., Intercomparison of meteorological analyses and trajectories in the Antarctic lower stratosphere with Concordiasi superpressure balloon observations, *Atmos. Chem. Phys.*, 17, 8045-8061, <https://doi.org/10.5194/acp-17-8045-2017>, 2017.

Boccara et al. did not investigate the reanalyses we used here.

Friedrich et al. reported that “Loon temperature measurements are not suitable for comparison with reanalyses”.

We have added a discussion of the Hoffmann et al results (not published at the time we submitted our manuscript) and Figure 18 to facilitate the discussion at the end of the results section (see below).

I would also suggest to rephrase “Independent datasets such as radiosondes, satellite observations,...”, simply because the data sets may have been subject to data assimilation at some of the centers and therefore might not be “independent” in a strict sense.

Data centers have also run “data denial experiments” which are independent in a strict sense so we have added an example for that process.

p5, L9: Add a reference for the MLS measurements?

We added Waters et al (2006) (already cited later in the paper).

p5, L10: So far I had not associated ESA with the “A-train” constellation?

We modified the text to refer simply to the “A-train”. “NASA”, “CNES” and “JAXA” are the space agencies responsible for coordination of the satellites in the A-Train. e.g. see [https://www.nasa.gov/mission\\_pages/a-train/a-train.html](https://www.nasa.gov/mission_pages/a-train/a-train.html).

p5, L19-30: Maybe summarize this information in a table? It might be worthwhile adding information on the vertical resolution of the data sets in the height range relevant for this study.

We have provided a table. We have added the vertical spacings for the reanalyses.

p6, L4-5: How was the interpolation performed, linearly with respect to  $\log(p)$ ?

Yes, this is now indicated in the revised text.

p6, L27-p7, L2: Maybe add a few words regarding the uncertainties of T\_STS (or say that this will be discussed later in the paper)?

We added the following text. “Estimated uncertainties in the reference point temperatures are discussed in Sections ...”

p7, L11: “Even though the RO measurements ‘per se’ are SI-traceable...” What does this mean?

The RO measurements are timing measurements of the phase delays of the signal along the atmospheric path from the GNSS transmitter to the LEO receiver. The phase delays are accurately calculated by reference to the international atomic time standard and as such are traceable to the SI second. We modified the text. “Even though the RO measurements of signal phase delays are traceable to the SI second, ...”

p7, L21-31: Not sure if this detailed explanation on how the noise was estimated is really needed? Maybe just summarize the findings of Staten and Reichler?

We prefer to retain this level of detail.

p8, L1: "...and -0.5K above 35 km" does not seem to be relevant for this study?

Although not directly relevant, it does no harm either to point out that the RO accuracy becomes worse above the region studied.

p8, L9-12: What are typical values of  $z_{Ttop}$ ,  $z_{Sbot}$ , and  $H_{Sbot}$ ? Naively, I was thinking  $z_{Ttop}$  and  $z_{Sbot}$  are the same?

$z_{Ttop}$  is the top of the tropopause whereas  $z_{Sbot}$  is the bottom of the stratosphere and the gap in between is the tropopause transition layer (TTL). Typical values vary with latitude/season. Only  $z_{Sbot}$  is relevant for our study. We give values we found in the results section.

p8, L22-28: What is causing the differences between the "dry" and "wet" GPS profiles? The differences do not seem to be related to the water vapor correction at these height levels?

We used the "dry" profiles since they are appropriate for the extremely low moisture content of the atmospheric region above 100 hPa. However, since other studies have used "wet" instead of "dry" profiles in the same region we decided to report on the differences we found. Although we do not know the origin of the differences, the point is made that the differences are small enough that either "wet" or "dry" could have been used for this analysis... "The wet temperatures yield results that are consistent with the dry temperatures and therefore are not considered further in this paper."

p9, L20: Another prominent reference in addition to Doernbrack et al. is: Carslaw et al., Increased stratospheric ozone depletion due to mountain-induced atmospheric waves, *Nature*, 391, 675678, 1998.

We added the reference to Carslaw et al.

p11, L15-20: The patterns might also be compared with Hindley et al. (2015), who used COSMIC data:

Hindley et al., The southern stratospheric gravity wave hot spot: individual waves and their momentum fluxes measured by COSMIC GPS-RO, *Atmos. Chem. Phys.*, 15, 7797-7818, <https://doi.org/10.5194/acp-15-7797-2015>, 2015.

We added the reference to Hindley et al.

p11, L21-32: I found it a bit difficult to follow the text in this paragraph, in particular this sentence: "A decrease in the spread of the temperature differences of reanalysis data compared to COSMIC should be detectable by rejecting the temperature profiles from consideration that are expected to have lower fidelity to the true atmosphere." Maybe rephrase this sentence/paragraph a bit, using easier words? The message is (as I understood) that you are excluding those COSMIC profiles from the statistical analysis that contain gravity waves, because those are gener-

ally not captured well by the reanalyses because of their limited spatial resolution? This makes sense, I think, as it puts emphasis on the evaluation of the large-scale state.

Yes, you understood our intent correctly. We modified the explanation in the revised text as suggested. We also reference the Hoffmann et al (2017) study of Concordiasi balloon data.

“Small-scale temperature fluctuations cannot be captured accurately by the reanalysis data because of their limited spatial resolution. For example, a study of superpressure balloon measurements by Hoffmann et al (2017a) found that ERA-I, MERRA and MERRA-2 reproduced about 30% of the standard deviation of the balloon temperature fluctuations, whereas the lower spatial resolution NCEP/NCAR reanalysis reproduced only 15% and the higher resolution ECMWF operational analysis reproduced 60%. ECMWF analyses also underestimate both gravity wave momentum fluxes derived from the balloon measurements (Jewtoukoff et al., 2015) and wave amplitudes derived from Aqua AIRS (Hoffmann et al., 2017b). Similarly, the COSMIC data should perform better than the reanalyses because of their higher resolution.”

p12, L4: I would suggest to add 1-2 sentences regarding the motivation for the orographic case study at the begin of this section. Reading the paper the first time, I found it a bit strange that at the end of Sect. 4.1 you are saying you are excluding gravity wave-affected data from the analysis and then the next section is showing a gravity wave case study.

A brief statement was added.

Overall, the case study is very interesting, I think, as it clearly illustrates the difficulties related to the representation of gravity waves in reanalyses data. Perhaps the findings could be put into context with other recent work discussing this aspect? The studies listed below might be worthwhile considering. They found that meteorological analyses and forecasts generally tend to show both orographic and non-orographic gravity waves patterns in the correct locations. However, wave amplitudes are significantly underestimated and wavelengths are overestimated (as can be seen also in your Fig. 4), which is attributed to the limited spatial resolution or truncation of the forecast models.

Schroeder et al., Gravity waves resolved in ECMWF and measured by SABER, *Geophys. Res. Lett.*, 36, L10805, doi:10.1029/2008GL037054.

Jewtoukoff, et al., Comparison of Gravity Waves in the Southern Hemisphere Derived from Balloon Observations and the ECMWF Analyses. *J. Atmos. Sci.*, 72, 34493468, <https://doi.org/10.1175/JAS-D-14-0324.1>, 2015.

Hoffmann et al., A decadal satellite record of gravity wave activity in the lower stratosphere to study polar stratospheric cloud formation, *Atmos. Chem. Phys.*, 17, 2901- 2920, <https://doi.org/10.5194/acp-17-2901-2017>, 2017.

Hoffmann et al., Intercomparison of meteorological analyses and trajectories in the Antarctic lower stratosphere with Concordiasi superpressure balloon observations, *Atmos. Chem. Phys.*, 17, 8045-8061, <https://doi.org/10.5194/acp-17-8045-2017>, 2017.

The case study was chosen simply based on a striking observation of correlated ice PSCs and cold phases. The responses of the reanalyses shown in Fig 4 do vary to a surprising extent and, although we should be wary of general conclusions based on one sample, their spatial resolutions appear to be correlated in the way expected.

We have added a brief discussion in the text concerning the points you raised...

“In the rest of this paper we concentrate on the large-scale temperatures, facilitated by the effective low-pass filtering using the  $E_p$  threshold to remove gravity-wave fluctuations. However, further work on issues related to the representation of gravity waves in the reanalyses would be worthwhile, and the high-pass side of the  $E_p$  threshold may provide useful insights.”

p12, L11-15: Which height level are the wind speeds of 25-35 m/s referring to? For estimation of gravity wave vertical wavelengths by means of the dispersion relation the winds at the observational level should be considered. There might be significant Doppler shifting and change in wavelength towards longer wavelengths if the stratospheric winds are stronger than the low-level winds.

We modified the text to indicate the height is that of the ice PSCs. “... the wind direction is almost orthogonal to the ridge line, with wind speeds  $u \sim 25\text{--}35 \text{ ms}^{-1}$  corresponding to the observation of ice clouds in the pressure range 80–40 hPa.”

p12, L18-20: Are these differences in wave amplitude correlated with the horizontal resolution of the reanalyses data sets?

Yes, NCEP-CFSR has the highest horizontal resolution and ERA-I the lowest compared to the other reanalyses. We have modified the text accordingly.

“At 50 hPa the peak to trough temperature differences are 7.4, 6.2, 8.0, 10.0, 6.1 and 14.9 K for GEOS-5.9.1, MERRA, MERRA-2, JRA-55, ERA-I and NCEP-CFSR, respectively; i.e., over a factor of two difference is seen in the temperature amplitudes between the reanalyses. These differences in the wave amplitudes are rather well correlated with the spatial resolutions of the reanalyses (see Table 1).”

p13, L11-15: How do these findings regarding the biases of the reanalyses relate to other studies on the topic? Earlier studies found quite significant warm or cold biases of reanalyses data (varying with height) in the polar winter stratosphere, I think.

This is now discussed at the end of the results section.

“Recently, Hoffmann et al. (2017a) used superpressure balloon measurements made during the Antarctic Concordiasi campaign in September 2010 to January 2011 to validate meteorological analyses and reanalyses. Over the flight paths of the balloons (17–18.5 km (58.2–69.1 hPa) and 60° S – 85° S), Hoffmann et al. found warm biases ranging from 0.6 to 1.5 K for ERA-I, MERRA and MERRA-2, increasing towards the pole, and standard deviations of 0.5–0.8 K, with ERA-I showing smaller standard deviations than MERRA. Whereas Hoffmann et al. find MERRA to be the warmest and ERA-I the coldest, we find the opposite order compared to the

COSMIC and thermodynamic temperature references (see Figure 16). Also we find negative temperature biases for MERRA and MERRA-2 and only a slight positive bias for ERA-I, with no significant latitudinal gradients (Figure 6). To reconcile this apparent discrepancy we show daily mean temperatures (at 12UT) for MERRA and MERRA-2 relative to ERA-I in Figure 18 and highlight the non-overlapping time periods of the PSC analysis window (green line) and the balloon flights (red line). Clearly, measurements in the later time period of the balloon flights (September-December) sample different atmospheric conditions than experienced in the earlier time period (May-August). Differences between reanalysis temperatures along the individual balloon trajectories are likely to be amplified compared to the differences in mean polar cap temperatures.

As we noted previously MERRA does not assimilate COSMIC data, whereas MERRA-2 and the other reanalyses we investigated do assimilate COSMIC data, and hence some of the reduction in the bias of MERRA-2 compared to MERRA seen in Figure 18 is likely to be attributable to the use of GPS RO data in the former.

Large vertical oscillations of up to  $\pm 2-3$  K were reported in the differences between ECMWF operational analyses and the CHallenging Minisatellite Payload (CHAMP) RO data in the 2002 to 2006 June-August Antarctic polar vortices (Gobiet et al (2005), Gobiet et al (2007)). Similar height-dependent features were also found (Parrondo et al 2007) in comparisons of ECMWF analyses with radiosondes. The value of the RO dataset as a reference was ably demonstrated by comparisons of CHAMP RO with ECMWF and other meteorological data (GEOS-4, MetO, NCEP/CPC, NCEP Rean) for June-August 2003 (Gobiet et al 2007). None of the other dataset differences showed features consistent with ECMWF, nor were any two consistent with each other, e.g. GEOS-4 displayed an Antarctic cold bias relative to CHAMP at 25–30 km, whereas NCEP Rean displayed a warm bias in roughly the same range. The absence of spurious vertical features in the comparisons we have presented here underlines the general much closer agreement amongst the more modern reanalysis systems.”

p13, L18-19: I am not so familiar with the CALIOP classification of PSCs. Do MIX1, MIX2, and MIX2-enh include or are mainly dominated by NAT?

All the CALIOP MIX classifications include NAT (detected by the above threshold non-zero depolarization signal) and the ubiquitous STS. Although STS may be the dominant component, whenever NAT is present (above the detection threshold) the classification is reported as a MIX type. From simulations (see Fig 10, Pitts et al 2013) the NAT number densities are  $< 10^{-3} \text{ cm}^{-3}$  for MIX1,  $10^{-3}$  to  $10^{-1} \text{ cm}^{-3}$  for MIX2 and  $> 10^{-1} \text{ cm}^{-3}$  for MIX2-enh. The STS classification therefore means that no NAT is detected above the detection threshold.

p14, L19-p15, 12: Section 4.6 does not seem to present any results, but recapitulates the method? Maybe merge with Sect. 4.7?

Section 4.6 was a summary of the procedure we followed. Following the suggestion of referee RC2 we moved the text to the methods section.

p16, L13-16: I would not directly expect the distance of reanalysis grid points to observations being a reason for causing two distinct modes of temperature precision because I would expect those distances to vary continuously over the study area?



Satellite observations would drift through all grid points as you indicate. However, against this background there may be radiosonde observations recurring in practically static locations close to the grid points.

p17, L15-16: I am afraid, do not fully understand this sentence: "The standard deviations result from the combination of the quadrature addition of the precisions of the reanalyses and the reference points. "What does 'precision' of the reference points" refer to?

We mean the precision of the reference point temperatures as estimated in Figs 1c and 2c.

p18, L24-25: However, the standard deviations with respect to the reanalyses are only similar, because gravity wave-affected profiles showing small-scale temperature fluctuations have been excluded in your analysis, right? It might be good to repeat this here.

This is correct, but the data with detected gravity waves constitutes only about 4% and 12% for SH and NH respectively as stated in the text. Excluding these small fractions probably does not reduce the standard deviations much. We indicated in the revised text that we are effectively applying a low-pass filter to examine the large-scale temperature structure.

p19, L8-9: I would agree that this study showed much better agreement between the reanalyses and observations than earlier work. However, I am not sure if you really demonstrated that point in the paper (see also comment regarding p13, L11-15)? The discussion of this aspect could be extended a bit.

This is now discussed at the end of the results section.

p31, Fig. 3: Maybe indicate the noise variance of the COSMIC data in Figs 3a and 3d? In the caption the unit "K<sup>2</sup>" is missing in a few places, e.g. "0.1" – > "0.1 K<sup>2</sup>" and so on.

The estimated noise variance is about 0.03 K<sup>2</sup>. We also fixed the units in the caption.

p33, Fig. 5: Does this analysis consider filtering of small-scale fluctuations due to gravity waves? There seem to be notable differences in the medians between the reanalyses. Is this related to COSMIC data being or not being assimilated in some of the reanalysis? How do these results compare to other studies?

Yes, the same gravity wave threshold as in Fig 3 is applied here. We indicate this at the end of the section on the wave case study. Only MERRA does not assimilate GPS-RO and this does have an appreciable effect on the median values in the SH and NH. We find little variation of the medians and standard deviations over the latitude range and comment on this at the end of the results section.

#### Technical Corrections

p11, l4: Remove units "J Kg<sup>-1</sup>" from equation (3)? And "Kg" should be "kg" in other places?

Ok.



p12, L10: peninsula – > Peninsula (maybe use either “Palmer Peninsula” or “Antarctic Peninsula” throughout the manuscript for consistency?)

Palmer is now used throughout.

p12, L11: lambda\_v – > lambda\_z

Ok.

p14, L31: ERA-I – > ERA-Interim (and in other places)

We prefer to use ERA-I in the text for consistency with the figures and therefore instead substituted ERA-Interim – > ERA-I

p36, Fig. 8 and p37, Fig. 9: y-axis labels are partly missing

The 2nd and 3rd rows are successive enlargements of a region in the 1st row of images centered at 32 hPa. The x by y dimensions in km are given in the text. y-labels indicating the pressure would not add useful information.

p44, Fig. 16: fix “standard (triangles) deviations”

The caption now reads “Median deviations (diamonds) and standard deviations (triangles)...”

## RC2 General Comments:

The authors present an evaluation of stratospheric temperatures at high latitudes in reanalyses by using temperatures from different satellite based observations including Microwave Limb Sounder (MLS) and GPS radio occultation (RO) measurements. They furthermore use observed regimes of different types of Polar Stratospheric Clouds (PCSs) for deriving temperature references based on the thermodynamics of supercooled ternary solutions and ice clouds.

The paper is well written but overall it is quite lengthy and includes 21 figures. At several places the content could easily be condensed and streamlined without losing information and thus presented in a more compact way. A sincere restructuring of the text in some sections is recommended and a restructuring/merging of figures. Furthermore, clarifications are needed regarding the definition of precision and accuracy, the choice of pressure levels, and the description of comparison methods (please see comments below).

I recommend publishing the manuscript after revision taking into account the reviewers recommendations and providing necessary clarifications. Please find a list of major and minor comments below

We will address the concerns of the referee in the modified manuscript. We reply to specific comments below.

## RC2 Major Comments:

Abstract: The abstract is much too long and definitely should be shortened by half. Only essential information and results should be stated. E.g., line 10 to 16 on page 2 could be deleted. Is the statement on GPS RO uncertainties correct: “accuracy  $< 0.2$  K, precision  $> 0.7$ K” (also in paper text and conclusion section)? To my knowledge it should be vice versa. The precision is about 0.25 K and the accuracy in the tropopause region about 0.7 K increasing exponentially in the stratosphere (see also comment below).

The abstract has been shortened to a reasonable length.

Your comments on accuracy vs precision for GPS-RO appear to be incorrect according to the literature on the RO measurement technique, which we cite in some detail on pages 7 and 8. We note that it is the precision (standard deviation) that increases exponentially in the stratosphere, whereas the accuracy (bias) is almost constant. Figs 18f and 19f indicate very good agreement with the standard GPS RO model error given in Eqn 1.

Methods:

Computation of pressure levels:

“The synoptic gridded reanalysis temperatures are interpolated to a common vertical pressure grid (100-10 hPa), with 6 levels per decade ...” Why are the pressure levels chosen this way for the reanalyses and the radio occultation observations, e.g., levels of 61 hPa or 46 hPa, etc.? Is there a specific reason for this? I strongly recommend using standard pressure levels or pressure levels with 10 hPa steps, i.e., plain numbers, as used later in the manuscript anyway. What

does “fixed pressure levels per decade” mean? “For convenience we interpolated the COSMIC temperature profiles to a set of fixed pressure levels with 24 levels per decade ..., approximately 2/3 km vertical resolution.” Please revise the last statement.

The “odd looking” pressure levels are a subset of those chosen by the Aura science team for all instruments on the Aura platform. The pressure levels,  $p(i)$ , are defined as a fixed number of levels,  $n$ , per decade change in pressure (i.e.  $p(i) = 10^{i/n}$ ) so they are in a logarithmic series. This is necessary because the MLS measurements cover a large region of the atmosphere and therefore linear 10 hPa pressure steps are not practical for the MLS instrument.

The MLS data processing retrieves products on either a low resolution  $n = 6$  levels per decade pressure grid (e.g. for HNO<sub>3</sub>, N<sub>2</sub>O) or higher resolution  $n = 12$  levels per decade pressure grid (e.g. for temperature, H<sub>2</sub>O, O<sub>3</sub>). Note that the levels have a structure similar to the well-known E-series (E6 and E12) of preferred values for electrical components such as resistors.

Since GPS-RO and reanalyses are of higher vertical resolution than the MLS grids, it is appropriate to interpolate both of these to the MLS low resolution pressure grid. We use the 6-level per decade grid since our definition of thermodynamic reference temperatures is limited by its dependence on the low resolution HNO<sub>3</sub> data.

In the gravity wave case study. We use the native NCEP-CFSR reanalysis levels 100, 70, 50, 30, and 20 hPa since the complications of the CALIOP/MLS field of view are not involved in this section. The MLS H<sub>2</sub>O data are instead interpolated to the reanalysis grid.

The vertical resolution of GPS RO observations ranges from a 0.5 km (100 m in case of wave optics processing) in the troposphere to about 1.5 km in the stratosphere. By interpolating the vertical levels you change the sampling of the height/pressure levels.

The atmPrf GPS-RO temperatures are supplied on a vertical grid with spacing of about 20m. In the separate analysis used for gravity waves the GPS-RO data are interpolated to a high resolution pressure grid (24 levels per decade) with approximately 2/3 km vertical spacing.

#### Section 2.4:

Please explain explicitly how the reanalyses are compared with the radio occultation observations. As I understand you compare the gridded reanalyses data with individual COSMIC temperature profiles (supposedly averaged in the respective grid or zonal mean). Doing it this way you would not account for the different sampling of the observations. A comparison should be either performed by subsampling the reanalyses at the locations of the RO observations (i.e., comparing colocated profiles) or by comparing monthly-mean zonal-mean reanalyses data with zonal-mean sampling error corrected RO climatologies.

We do actually compare colocated profiles. Unfortunately, we omitted this important detail of the reanalysis vs COSMIC comparisons from the original manuscript. The sampling of the reanalysis gridded data for the GPS-RO measurements is done the same way as for the MLS temperatures as indicated in Section 2.1 ...

“The synoptic gridded reanalysis temperatures are interpolated to a common vertical pressure grid (100–10 hPa), with 6 levels per decade ( $p = 100 \times 10^{i/6}$ ;  $i = 0, 1, \dots, 6$ ), and to the MLS measurement times and geophysical locations.”

This creates a colocated set of reanalysis and MLS profiles. A different set of colocated profiles is created from the reanalysis and COSMIC data. We amended the text to reflect the similar treatment of GPS and MLS. Note that we do not try to obtain colocated MLS and GPS profiles.

Cite Schreiner et al. (2007; doi:10.1029/2006GL027557) in section 2.4 as they made the first analysis on the precision of COSMIC data. Their results were confirmed by Alexander et al. (2014), who derived a precision of about 0.1% in refractivity between 8-25 km (larger above 30 km) which translates to about 0.25 K. No strong dependence of the estimated precision on latitude or season was found.

We added the citation to Schreiner et al. “Schreiner et al (2007) investigated the precision of the COSMIC data by leveraging the close configuration of the six satellites during the early deployment phase of the mission.” We have already cited Alexander et al and others in the same section. Also from Alexander et al., we noted that between 10 and 30 km the temperature bias was found to be +0.1 K i.e. almost a constant value for accuracy with height.

Is this consistent with your statement in the abstract and conclusion section on precision and accuracy?

Yes.

Please include a definition of precision and accuracy in the method section before values for the different data sets are discussed and give an explicit description on how precision and accuracy are computed in your study.

We use standard definitions of accuracy and precision. (i) high accuracy is determined by the narrowness of the spread of repeated measurements relative to the underlying true value. (ii) high precision is determined by the narrowness of repeated measurements with respect to a measure of their central value such as the mean or median. Therefore the mean of a set of precise measurements may have a large deviation (bias) from the true value, although the standard deviation (about the mean) of the precise set may be small. High accuracy measurements have by definition a small bias and small standard deviation.

In this study we use the GPS-RO temperatures because of their previously validated high accuracy and precision. We also use the reference temperatures calculated from the thermodynamics of PSC formation.

Details are given in the “Datasets and methodology” section...

“The accuracy (bias) of the reanalysis temperatures are obtained relative to the reference temperatures (LIQ, ICE, and COSMIC). We use the calculated standard deviations of the temperature differences to estimate the measurement precisions i.e. high precision is determined by the narrowness of repeated measurements with respect to a measure of their central value such as

the mean or median.”

Move method descriptions from the results section to the method section (see comments below on restructuring).

All suggestions on restructuring the manuscript have been followed where possible.

### **Structure of the manuscript:**

Introduction:

Page 4, 3rd paragraph: This paragraph already describes the methodological approach in some detail and would rather fit at the beginning of the method section.

Ok.

Page 4, line 29: “However, lack of sufficient statistics in the Arctic precludes a robust conclusion for ICE PSCs.” This is a result and the sentence should be moved to the conclusion section or/and the results section.

Ok.

Page 4, line 31-33: Detailed description of investigated dates should be moved to the beginning of the methods section.

Ok.

### **Method section:**

I recommend slight restructuring: Start with the reanalyses description. The information in the first paragraph does not really fit here at the beginning and should be moved to sections 2.2 where CALIOP observations are described and to section 2.3 where MLS is described.

Ok.

Section 2.1: The information on all the reanalyses could be summarized in a Table and would give a more compact overview.

A table has been provided.

Streamline page 7 and 8 as you recapitulate several studies in quite a lengthy way.

We prefer to retain this level of detail.

Results sections:

The results sections include method descriptions such as section 4.6 describing how the comparison of reanalyses temperatures to LIQ and ICE reference points is performed and in section 4.8.2 (last paragraph) on difference computations. These method descriptions should be moved to the method section.

Ok.

Furthermore some results sections are very short and could be merged into one section such as sections 4.4, 4.5, and 4.7. There is no need to make a separate section for each figure but rather to comprise related topics in one section. The merged section 4.4 could be entitled, e.g., “PSC types from CALIOP and their representation in MLS observations”.

Ok.

Section 4.8 Polar temperature reference points:

Remove sub-sub-sections and streamline the text.

Ok, minor sub sections were removed.

Section title could be “Reanalysis temperatures compared to LIQ and ICE temperature reference points”

Ok.

Figures:

General: You often provide the same information twice in the figure captions and in the description of figures in the text. Please give the technical description of the figure in the caption and provide explanations and description of the scientific results in the text, e.g., Fig. 13.

Some information is repeated in the caption so the reader does not have to flip back and forth between the text and the figure.

Fig. 5: The latitudinal structure from 60S/N to 90S/N is rather uniform for the median and the standard deviation. A structure in temperature differences is mainly visible in the vertical domain. Averaging over 60S-90S and 60N-90N would give a condensed overview. Median and standard deviation profile could be shown in one panel. Fig. 5 could be condensed in 2 rows for the Arctic and Antarctic. In Figure 6 the information on latitudinal differences and vertical differences is given again, anyway.

We prefer to retain the format of Fig 5. As you note, the structure is immediately visible in this presentation format. In addition we now refer to this figure in the discussion of comparisons with a recent paper by Hoffmann et al. (see response to RC1 above).

Fig. 6: The vertical boxes should also be centered around a zero line as done for the latitudes.

There is no zero-line for the vertical scale.

Fig. 9: Please condense information. Fig.9a is the same Figure as already shown in Fig. 8. Fig.9b does not really give much information, it can be stated in the text. Please check whether this figure is really needed or the information could be stated in the text.

Fig. 9 has been deleted. Essential information was placed in the text instead.

Fig. 11: What is the reason for showing the information twice? Why do you show inverse temperature? It is distracting to the reader unless there is a specific reason for it. I suggest plotting a logarithmic y-axis, using temperature for the x-axis, and showing only 2 plots in Fig. 11.

We believe it is helpful to show both diagrams (a) because of the continuity with Fig 2 and (b) because of the high degree of linearization that results from the transformation to log mixing ratio vs  $1/T$  (see Murphy and Koop, QJRMS (2005), doi: 10.1256/qj.04.94).

Fig. 12: Suggest having a similar design as for Fig. 11, i.e., plotting the temperature axis from 175 K to 200 K and removing the inverse temperature x-axis.

Again, this plot format is used because  $\log(\text{PICE})$  vs  $1/T$  has a linear relation (black/blue dashed line).

Fig. 18 and 19: The standard deviations (Fig. 18.d-f) could be easily plotted in Fig. 18 a-c by extending the x-axis to -3K to 3K. The same could be done for Fig. 19. Fig. 18 and 19 could then be merged to one Fig. showing SH in the upper panels and NH in the lower panels. So the reader would be provided with compact information.

The figures were designed to be quite easy to read in their current format and we prefer not to squash the space along the x-axis in order to cram more plot lines together.

Fig. 14 and 15: Please compile the information printed in the different panels in a Table. Fig. 14 and 15 could be removed and information of section 4.8.1 could be streamlined. The description at page 16, line 10 to 18, could be removed and the main information stated in one sentence.

Figures 14 and 15 were removed. The information is now supplied in Tables 1 and 2. The description on the possibility of more than one mode has been retained.

Minor comments:

The title is very long and contains 5 acronyms. It should be shortened. I think it is not necessary to list all the sensors explicitly in the title, could be replaced by “satellite observations”.

We prefer to retain the acronyms in the title as they provide simple built-in keywords for search engines whereas “satellite observations” is far too vague.

Also the term “supercooled ternary solutions” might not be a familiar term for many readers. Maybe use “polar stratospheric cloud types or polar stratospheric cloud regimes” instead.



We prefer to retain the kind of PSCs in the title. “Supercooled ternary solution” has been in use for over 30 years.

Reanalysis: More than one reanalysis is evaluated, rather use “reanalyses” in the title.

We have modified the title. “Accuracy and precision of polar lower stratospheric temperatures from reanalyses evaluated from A-train CALIOP and MLS, COSMIC GPS RO, and the equilibrium thermodynamics of supercooled ternary solutions and ice clouds.”

Page 2, line 19: “significant low bias in MLS temperature of up to 3 K” ? Do you mean “large bias”?

No, we mean low bias. MLS temperatures are lower by up to 3 K.

Page 2, line 31: What does “(one-off research satellites)” mean, check singular/plural.

We changed “one-off” to “one-of-a-kind”. This refers to any kind of satellite instrument (such as MLS, MIPAS etc) that is not part of a long-term dedicated series of operational satellites (such as NOAA GOES).

Page 2, line 32: What is “temperatures measured with the Geophysica”: Please be explicit. What is the Geophysica, how were the temperatures measured, state the instrument?

The Geophysica is a high-altitude research aircraft and ambient temperatures were measured by the Thermodynamic Complex instrument (Shur et al., 2006). We do not see the need to include this reference.

“Wegner et al (2012) showed a comparison of ERA-I Arctic temperatures in March 2005 that indicates a 1.5 K warm bias in ERA-I below 205 K compared to the ambient temperatures measured with the Geophysica high-altitude research aircraft.”

Page 6, line 26: “-2-0 K” change to “-2 K to 0 K”

Ok.

Page 7, line13: “requires a number of assumptions because of the long ray path through a nonuniform atmosphere. Therefore, corrections are required for ionospheric effects, variations in water vapor, and gradients in in temperature along the ray path.” This statement is not fully correct. Please reformulate/clarify.

Initialization (of bending angles) at high altitudes is performed where the signal to noise ratio of the measurement becomes low. An ionospheric correction is applied through differencing of the two GPS frequencies to remove the ionospheric contribution to the measurement and to gain information on the neutral atmosphere only. Refractivity then includes information on the dry and moist part of the atmosphere (see Smith and Weintraub formula, as you explain on the next page). In a dry atmosphere, temperature can be retrieved without any further correc-

tion or initialization. In a moist atmosphere, i.e., in the mid- to lower troposphere, additional background information is needed to separate temperature and humidity information (usually through a 1DVar retrieval).

The above description does not appear to identify what is not “fully correct” in our original statement and therefore we have not modified it.

However, as you investigate temperatures at high latitudes in the stratosphere, you can use dry temperatures only. The discussion on wetPrf temperatures can be removed as they are not used.

Others papers have used wetPrf for their studies and in fact we have repeated the entire analysis using the wetPrf data. We have also compared the COSMIC version 2013.3520 wetPrf and atm-Prf temperatures and have therefore reported their differences. The point is that the differences are small enough that either could have been used for this analysis as is now noted in the revised manuscript.

Page 7: line 34: Remove “similar results were obtained over data sparse (Pacific) and data dense (USA) regions”. This is distracting as one might think it is RO data sparse and dense regions (but RO has almost equal distribution globally) but actually it relates to observations assimilated into ECMWF.

Ok, removed.

Page 8, line 21,22: insert “about” before “14 km” and before “9 km”.

Ok, inserted.

Page 9, line 20: Why a pressure range of 68 to 21 hPa and not 70 to 20 hPa.

As discussed previously the pressure range quoted is for our standard MLS pressure levels.

Page 10, Eq.3: correct to “J kg<sup>-1</sup>” and through paper text.

Ok, corrected.

Page 11: “A decrease in the spread of the temperature differences of reanalysis data compared to COSMIC should be detectable by rejecting the temperature profiles from consideration that are expected to have lower fidelity to the true atmosphere.” What is meant by fidelity to the true atmosphere? The truth is actually not known. Rejecting observational profiles with higher variance will of course improve the difference between reanalyses and observations if observations show a higher variance than the reanalyses at high latitudes, which is well known for RO. I actually do not understand the purpose of rejecting profiles with higher variance.

“The truth is actually not known.” Quite true. However, we are able to reject specific reanalysis temperature profiles that are likely to be poorly represented because the model resolution cannot accurately capture gravity wave effects. We postulate that the remaining sample of reanalysis temperatures will be closer to the true temperatures (i.e. higher fidelity). We generate a proxy

for gravity wave activity at each GPS-RO location from the variance in the vertical structure of the COSMIC temperatures (80–20 hPa). If the variance is above a chosen threshold then we reject the matched reanalysis/COSMIC profile from consideration. We can see from Fig 3(c,f) that both the variance and mean difference between ERA-I and COSMIC are improved using this method. Fig 3(b,c) shows that this is not just some isotropic removal of “bad” high variance profiles at high latitudes since the geophysical structure reveals an association with known gravity wave “hot-spots”.

We have modified the explanation as also suggested by referee RC1.

Page 12, line 28: What do you mean with “the geophysical structure”? The vertical structure versus the latitudinal structure at high latitudes is shown.

Removed the word “geophysical”.

Page 13, line 2: Use clear wording in description of Fig. 6. Rather than saying the “box heights” it is the differences in the vertical between reanalyses and RO.

The terms box width and box height are defined on lines 6–7 of Page 13, these are used to simplify the description.

Page 13, line 22: Why do you show the 46 hPa level?

It is a representative level. Other figures also show the 46 hPa level: Figs 11, 14, 15, 16, and 17. Fig 13 displays 31 hPa because the HNO<sub>3</sub> range is larger than at 46 hPa.

Page 14, end of section 4.5: Please give percentage of scenes analyzed with respect to available scenes.

Only about 15% of the scenes containing STS or ice PSCs are accepted. This information was added to the text.

Page 17: The last part of section 4.8.2 (page 18, first paragraph) is very hard to read. Please reformulate and streamline info.

Yes, we agree the paragraph looks ugly, but we believe the math is correct.

Page 44, Fig. 16, caption: Correct to: “Median (diamonds) and mean (triangles)...” Section titles: Please remove Tre-Tro, Tre-Teq, and similar in section titles.

The caption now reads “Median deviations (diamonds) and standard deviations (triangles)...” Section titles were removed as part of the restructuring suggested above.

# Accuracy and precision of polar lower stratospheric ~~polar reanalysis~~ temperatures from reanalyses evaluated from A-train CALIOP and MLS, COSMIC GPS RO, and the equilibrium thermodynamics of supercooled ternary solutions and ice clouds

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## Abstract.

We investigate the accuracy and precision of polar lower stratospheric temperatures (100–10 hPa during 2008–2013) reported in several contemporary reanalysis data sets comprising two versions of the Modern-Era Retrospective analysis for Research and Applications (MERRA and MERRA-2), the Japanese 55-year Reanalysis (JRA-55), the European Centre for  
5 Medium-range Weather Forecasts (ECMWF) interim reanalysis (~~ERA-Interim~~ERA-I), and the National Oceanic and Atmospheric Administration (NOAA) National Centers for Environmental Prediction (NCEP) Climate Forecast System Reanalysis (NCEP-CFSR). We also include the Goddard Earth Observing System Model version 5.9.1 near real-time analysis (GEOS-5.9.1). Comparisons of these datasets are made with respect to retrieved temperatures from the Aura Microwave Limb Sounder (MLS), Constellation Observing System for Meteorology, Ionosphere and Climate (COSMIC) Global Positioning System  
10 (GPS) Radio Occultation (RO) temperatures, and independent absolute temperature references defined by the equilibrium thermodynamics of supercooled ternary solutions (STS) and ice clouds. Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) observations of polar stratospheric clouds are used to determine the cloud particle types within the Aura MLS geometric field of view. The thermodynamic calculations for STS and the ice frost point use the colocated MLS gas-phase measurements of HNO<sub>3</sub> and H<sub>2</sub>O. The estimated accuracy and precision for the STS temperature reference, over the 68 to  
15 21 hPa pressure range, is 0.6–1.5 K and 0.3–0.6 K, respectively; for the ice temperature reference they are 0.4 K and 0.3 K, respectively. These uncertainties are smaller than those estimated for the retrieved MLS temperatures and also comparable to GPS RO uncertainties (accuracy < 0.2 K, precision > 0.7 K) in the same pressure range.

We examine a case study of the time-varying temperature structure associated with layered ice clouds formed by orographic gravity waves forced by flow over the Palmer ~~peninsula~~Peninsula, and compare how the wave amplitudes are reproduced  
20 by each reanalysis data set. We find that the spatial and temporal distribution of temperatures below the ice frost point, and hence the potential to form ice PSCs in model studies driven by the reanalyses, varies significantly because of the underlying differences in the representation of mountain wave activity. ~~We have therefore used temperature variances, calculated from the COSMIC GPS RO temperature data (80–20 hPa), and imposed a variance threshold to selectively remove profiles with suspected enhanced wave activity. We examine the resulting improvement to the fidelity of the reanalysis temperatures.~~

~~High-accuracy~~ High-accuracy COSMIC temperatures are used as a common reference to intercompare the reanalysis temperatures and, although the COSMIC data are routinely assimilated by each reanalysis scheme except for MERRA, we find that there are significant departures from uniformity in the structure of the meridional and altitude temperature differences. Over the 68–21 hPa pressure range, the biases of the reanalyses with respect to COSMIC temperatures for both polar regions fall within the narrow range of  $-0.6$  K to  $+0.5$  K. ~~The corresponding standard deviations of the differences are  $\sim 0.8$  K at 100 hPa and increase exponentially with altitude, as expected because of the gradually worsening GPS-RO measurement precision.~~ GEOS-5.9.1, MERRA, MERRA-2 and JRA-55 have predominantly cold biases, whereas ERA-I has a predominantly warm bias. NCEP-CFSR has a warm bias in the Arctic, but becomes substantially colder in the Antarctic.

~~For the comparisons of the reanalysis temperatures with the thermodynamically calculated temperature references, we use the concept of an instrument field of view (FOV) fill-fraction. The distribution of CALIOP PSC types within the MLS geometric FOV are used to mitigate the effects of disparate types of PSCs occurring in the much larger MLS sample volume. This removes the speckle effect that arises either because of uncertainty in the detection classification from random noise in the CALIOP signals or from the microphysical effects of small-scale temperature fluctuations on the formation of PSC particles. We select viewing scenes with the requirement that 75% or more of the MLS geometric FOV is filled with CALIOP PSC detections of the same PSC type classification. Scenes satisfying this requirement for CALIOP STS detections we denote as LIQ, and for CALIOP ice detections we denote as ICE. Reanalysis temperatures are also compared with the PSC reference temperatures.~~ Over the 68–21 hPa pressure range, the reanalysis temperature biases are in the range  $-1.6$  K to  $-0.3$  K with standard deviations  $\sim 0.6$  K for the LIQ CALIOP STS reference, and in the range  $-0.9$  K to  $+0.1$  K with standard deviations  $\sim 0.7$  K for the ICE CALIOP ice reference. Comparisons of MLS temperatures with the LIQ and ICE PSC reference temperatures reveal vertical oscillations in the MLS temperatures, and a significant low bias in MLS temperatures of up to 3 K.

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## 25 1 Introduction

Over the last couple of decades, global reanalysis datasets have become one of the workhorse tools of the climate research community for understanding atmospheric processes and variability (Fujiwara et al., 2017) and more recently for potentially investigating climate changes (Thorne and Vose, 2010; Dee et al., 2014; Simmons et al., 2014). A reanalysis system combines observations with predictions from a global forecast model that propagates information forward in time and space using an assimilation scheme to produce a control-weighted blend of the observations and the new forecast. Unlike operational analysis schemes, which are updated as needed to improve numerical weather prediction (NWP) capabilities, reanalysis systems are designed to be conservative and retain the same code-base, with the aim of producing consistent and low-artifact output content over their entire multi-decade timeseries for a given product version generation.

The state-of-the-art of NWP and reanalysis data has improved greatly over the years as computational technology has evolved and new observation systems, such as global navigation satellite system (GNSS) radio occultation (RO) and data from other advanced satellites (including ~~one-off~~ one-of-a-kind research satellites), have also been brought within the realm of data assimilation. Currently, there are numerous NWP centers that produce reanalysis products. Understandably, there are  
5 differences in the technical implementation of the highly complex reanalysis schemes between the NWP centers, and these can lead to differences in the reanalysis products. Accordingly, there is a need for the research community to know how the deficiencies of a particular reanalysis may impact their investigations. The SPARC (Stratosphere-troposphere Processes And their Role in Climate) Reanalysis Intercomparison Project (S-RIP) (Fujiwara et al., 2017) is a coordinated activity with the aim of understanding the underlying causes of differences among global reanalysis data products to help support the needs  
10 of the research community. Comparisons of reanalysis data with independent observations form an indispensable part of this assessment, and a core component of the evaluation process is to use satellite observations as a reference.

The focus of this paper is on the “Polar Processes” theme of the upcoming associated S-RIP report outlined by Fujiwara et al. (2017), in particular the intercomparison of reanalysis temperatures, and we seek to answer the question “*Can the thermodynamics of ~~supercooled ternary solutions and the ice frost point~~ polar stratospheric clouds be used to provide an absolute  
15 temperature reference in the polar regions?*”. Thermodynamic properties dictate that only two types of polar stratospheric cloud particles are conducive for this application: supercooled ternary solutions and water ice. As discussed in detail in Section 3, PSCs composed of nitric acid trihydrate particles are not suitable because they are often out of equilibrium with the ambient  $\text{HNO}_3$ . Polar processes, such as the potential for ozone loss via heterogeneous reactions (Solomon, 1999; Solomon et al., 2015), depend critically on temperature. The potential ozone loss is related to the volume of stratospheric air that is below  
20 certain critical temperature thresholds associated with formation of PSCs (Rex et al., 2004; Orsolini et al., 2009; Harris et al., 2010). Mean winter temperatures in the Arctic stratosphere are significantly higher than those in the Antarctic (e.g. Waugh and Polvani, 2010), such that the propensity for the formation of persistent Arctic PSCs is much lower, and the development of widespread synoptic ice PSCs is quite rare (Engel et al., 2013). Since the results of polar modeling studies are especially susceptible to errors in the underlying temperature fields, Chemistry–Climate Models (CCMs) (Butchart et al., 2011) are preferably  
25 used in a specified-dynamics (SD) mode for studying polar processes. In the SD-mode, CCMs are constrained by using Newtonian relaxation to nudge the model output at each time step towards the reanalysis temperatures and wind fields (e.g. Whole Atmosphere Community Climate Model (WACCM), Wegner et al., 2013)), and are therefore adapted better to represent polar winters with unusual ~~characterities~~ characteristics such as split vortices, exceptionally cold conditions, sudden warmings, etc. Accurate temperatures are critical, not only to process studies, but also to assessment of trends in stratospheric winter  
30 conditions, especially considering the prospects of an increased frequency of future episodes of severe Arctic ozone depletion (Rex et al., 2006; Sinnhuber et al., 2011; Langematz et al., 2014), following the record low seen in 2011 (Manney et al., 2011). A temperature difference of less than 1 K can have a significant effect on the outcome of model runs that are driven by reanalysis data. Errors in the extent of heterogeneous processing, arising from temperature biases, result in under/over estimate of activated chlorine, thus leading to too little/much chemical ozone loss. Temperature adjustments have often been applied in  
35 order to better match model predictions with observations (e.g. Danilin et al., 2000). Wohltmann et al. (2013) found a discrep-

ancy in modeled and observed HCl and ClO which could be improved by adjusting the reanalysis temperatures by  $-1.0$  K for ERA-I in the Arctic 2009/2010 winter. Brakebusch et al. (2013) found an improvement in modeled ozone loss with a  $-1.5$  K adjustment for an unspecified version of GEOS5 in the Arctic 2004/2005 winter. Wegner et al. (2012) showed a comparison of ERA-I Arctic temperatures in March 2005 that indicates a  $1.5$  K warm bias in ERA-I below  $205$  K compared to the [ambient](#) 5 temperatures measured with the Geophysica [high-altitude research aircraft](#). Solomon et al. (2015) demonstrated that a  $-2.0$  K adjustment to the MERRA temperatures in the 2011 Arctic winter provides a better fit ~~to~~ [of](#) the zonally averaged [modeled](#) total column ozone [to the observations](#). Improved knowledge of the temperature biases in reanalysis data would enhance confidence in the attribution of model errors to the underlying physico-chemical properties of PSCs and heterogeneous reactions.

Several previous intercomparisons of analyses and reanalyses generated by various national centers have been carried out 10 (e.g. Manney et al., 1996; Pawson et al., 1999; Manney et al., 2003, 2005) to assess their accuracy and ultimate suitability ~~for~~ [specifically for stratospheric](#) polar studies. Independent datasets such as radiosondes, satellite observations, Global Positioning System (GPS) Radio Occultation (RO) (Nedoluha et al., 2007) and temperature sensors on long-duration balloons (Hertzog et al., 2004; McDonald and Hertzog, 2008) have also been used to assess reanalysis temperatures. [Data denial experiments, in which the analyses are compared with and without ingestion of a particular dataset, are often used to test assimilation systems](#) 15 [\(e.g. Bauer et al., 2014\)](#).

Historically, the uncertainties in polar reanalysis temperatures, especially for the southern hemisphere, have been higher than those in other regions of the globe, because of sparse coverage from conventional temperature measurements such as radiosondes (e.g. Gobiet et al., 2005; de la Torre Juárez et al., 2009). In recent decades, the augmentation of the coverage of polar regions by an increase in satellite missions, including assimilation of research satellite data, and notably the advent of 20 GNSS RO, has dramatically improved the situation (Wang and Lin, 2007). Lawrence et al. (2015) examined a 34-year record of polar processing diagnostics for MERRA and ~~ERA-Interim~~ [ERA-I](#) reanalyses. They documented the introduction of new data streams and noted better agreement in the post-2001 timeframe following the assimilation of Aqua Atmospheric Infrared Sounder (AIRS) and Geostationary Operational Environmental Satellite (GOES) radiances into both schemes.

[In section 2 we review the satellite instruments, reanalysis datasets, and methodology. In section 3 we review the equilibrium](#) 25 [thermodynamics associated with the formation of stratospheric ternary solutions and ice clouds. In section 4 we present and discuss the results of the comparisons. Finally, in section 5 we present the conclusions.](#)

## 2 [Datasets and methodology](#)

We confine our investigations to the temperature data over the past decade from six contemporary reanalysis datasets and introduce a novel analysis based on the thermodynamics of supercooled ternary solutions and the ice frost point to provide an 30 absolute temperature reference. Near-simultaneous and colocated measurements of nitric acid, water vapor and cloud phases are currently only afforded by the precise formation flying of two satellite instruments in the A-train. These are the Aura Microwave Limb Sounder (MLS) instrument, which measures the gas-phase species, and the Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) lidar, which is used to classify PSC types. The analysis presented refines and extends the



methodology used originally by Lambert et al. (2012) to investigate the temperature existence regimes of different types of PSCs. Supercooled Ternary Solution (STS) and ice PSCs are identified by the CALIOP lidar PSC classification ~~and combined with spatially and temporally collocated MLS and gas-phase abundances~~. We accumulate statistics on the existence regimes for STS and ice PSCs by using CALIOP to identify the presence of PSCs in the ~~near-simultaneous and collocated~~-MLS geometric field of view at the along track resolution (165 km by 2.16 km). MLS is used to obtain the ~~spatially and temporally collocated~~ ambient gas-phase H<sub>2</sub>O and HNO<sub>3</sub> volume mixing ratios. These are required to calculate the theoretical equilibrium temperature dependence of the STS (T<sub>eq</sub>) and ice (T<sub>ice</sub>) PSCs. We compare the observed and calculated temperature distributions of (a) the uptake of HNO<sub>3</sub> in STS, and (b) the ice frost point, for each reanalysis data set and for MLS temperature. ~~However, lack of sufficient statistics in the Arctic precludes a robust conclusion for~~

We select viewing scenes in which there is a distinct dominant PSC classification in a sample volume that is similar in size to the MLS gas-species resolution. The requirement is that 75% or more of the CALIOP pixels in the MLS geometric field of view (FOV) have the same PSC classification. Scenes satisfying this requirement for CALIOP STS detections we denote as LIQ, and for CALIOP ice detections we denote as ICEPSCs. This is discussed in detail in Section 4.4.

To summarize, our approach includes the following steps :

- 15 – Identify LIQ and ICE PSCs using the CALIOP lidar measurements.
- Accumulate the CALIOP PSC types (LIQ and ICE) at the MLS along-track resolution (165 km × 2.16 km), ensuring that the same PSC type is detected in at least 75% of the MLS field of view.
- Calculate the theoretical temperature dependence of STS (T<sub>eq</sub>) and ice (T<sub>ice</sub>) PSCs under equilibrium conditions using the spatially and temporally collocated MLS gas-phase HNO<sub>3</sub> and H<sub>2</sub>O measurements.
- 20 – Compare (a) calculated and observed HNO<sub>3</sub> uptake in STS and (b) ice temperature distribution vs the frost point with reanalysis data and MLS temperatures. ~~We also compare the Antarctic and Arctic reanalysis temperatures poleward of 60° with the COSMIC temperatures used as a common reference (Section 2.5~~
- Create LIQ and ICE temperature distributions for each reanalysis dataset (all sampled by interpolating to the MLS measurement times and locations) and additionally for MLS temperature.
- 25 – Calculate the median and mean temperature deviations from T<sub>eq</sub> and T<sub>ice</sub> and their standard deviations for LIQ and ICE classifications, respectively.

The accuracy (bias) of the reanalysis temperatures is obtained relative to the reference temperatures (LIQ, ICE, and COSMIC). We use the calculated standard deviations of the temperature differences to estimate the measurement precisions, i.e. high precision is determined by the narrowness of repeated measurements with respect to a measure of their central value such as the mean or median.

We investigate six Antarctic PSC seasons from 20 May (d140) to 18 August (d230) from 2008 to 2013 in the lower stratosphere (100 hPa–10 hPa) for latitudes poleward of 60° S. Similarly, in the Arctic we investigate five PSC seasons from 2 December (d336) to 31 March (d090) from 2008/2009 to 2012/2013 for latitudes poleward of 60° N.

In section 2 we review the satellite instruments, reanalysis datasets, and methodology. In section 3 we review the equilibrium thermodynamics associated with the formation of stratospheric ternary solutions and ice clouds. In section 4 we present and discuss the results of the comparisons. Finally, in section 5 we present the conclusions.

### 3 Datasets and methodology

The Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) dual-wavelength elastic backscatter lidar (Winker et al., 2009) flies on the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO) satellite launched in April 2006. The Microwave Limb Sounder (MLS) is onboard the Aura spacecraft launched in July 2004. CALIPSO and Aura are part of the NASA/ESA afternoon “A-train” satellite constellation at 705 km nominal altitude and 98° inclination, with daily near-global coverage attained in 14.5 orbits. The initial A-train configuration of the CALIPSO and Aura spacecraft from April 2006 to April 2008 resulted in an across-track orbit offset of ~200 km, with the MLS tangent point leading the CALIOP nadir view by about 7.5 minutes. Since April 2008, Aura and CALIPSO have been operated to maintain positioning within tightly constrained control boxes, such that the MLS tangent point and the CALIOP nadir view are collocated to better than about 10–20 km and about 30 seconds.

#### 2.1 Reanalysis temperature data

The reanalysis data used are from four analysis centers (NASA, NOAA/NCEP, ECMWF, JMA). Details pertaining to the S-RIP intercomparisons can be found in Fujiwara et al. (2017) and are summarized below in Table 1.

GEOS-5.9.1 : 0.625° by 0.5° : 3hr : Rienecker et al. (2011) : near real-time assimilation system : Goddard Earth Observing System Model, Version 5 : NASA Global Modeling and Assimilation Office (GMAO) MERRA : 0.666° by 0.5° : 6hr : Rienecker et al. (2011) : Modern-Era Retrospective analysis for Research and Applications : NASA GMAO 0.626° by 0.5° : 3hr : Bosilovich et al. (2015) : Modern-Era Retrospective analysis for Research and Applications Version 2 : NASA GMAO JRA-55 : 0.582° by 0.56° : 6hr : Kobayashi et al. (2015) : Japanese 55-year Reanalysis : Japanese Meteorological Agency (JMA) ERA-Interim : 0.75° by 0.75° : 6hr : Dee et al. (2011) : European Centre for Medium-range Weather Forecasts (ECMWF) interim reanalysis : ECMWF NCEP-CFSR : 0.5° by 0.5° : 6hr : Saha et al. (2010) : National Oceanic and Atmospheric Administration (NOAA) National Centers for Environmental Prediction (NCEP) Climate Forecast System Reanalysis : NCEP All the above except MERRA include GPS-RO data during the time period studied here GEOS-5.9.1 is a near real-time assimilation product provided to the NASA Earth Observing System (EOS) instrument science teams

The synoptic gridded reanalysis temperatures are interpolated in log pressure to a common vertical pressure grid (100–10 hPa), with 6 levels per decade ( $p = 100 \times 10^{-i/6}$ ;  $i = 0, 6$   $p = 100 \times 10^{-i/6}$ ;  $i = 0, \dots, 6$ ), and to the MLS measurement times and geophysical locations. A separate dataset of collocated reanalysis temperature profiles is also created for the COSMIC

measurement times and locations, with the COSMIC temperatures linearly interpolated in log pressure to the same 6 level per decade grid.

## 2.2 CALIOP PSC data

5 The CALIOP dual-wavelength elastic backscatter lidar (Winker et al., 2009) flies on the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO) satellite launched in April 2006. We use the CALIOP Level 2 operational dataset L2PSCMask (v1 Polar Stratospheric Cloud Mask Product) produced by the CALIPSO science team. The Level-2 operational data consist of ~~nighttime-only~~nighttime-only data and contain profiles of PSC presence, composition, optical properties, and meteorological information along the CALIPSO orbit tracks at 5 km horizontal by 180 m vertical resolution. We have applied  
10 post-processing to generate coarser horizontal/vertical bins for a better comparison at the scale of the MLS along-track and vertical resolution. Each averaging bin is the size of the MLS along-track vertical profile separation (165 km) and the height between the mid-points of the retrieval pressure levels (2.16 km) for the MLS HNO<sub>3</sub> data product. This we refer to as the MLS geometric field of view. There are approximately four hundred CALIOP 5 km x 0.18 km “pixels” within the MLS geometric field of view.

## 15 2.3 MLS gas-phase constituents and temperature

~~The Microwave Limb Sounder~~MLS is onboard the Aura spacecraft launched in July 2004 and measures thermal emission at millimeter and sub-millimeter wavelengths from the Earth’s limb (Waters et al., 2006) along the forward direction of the Aura spacecraft flight track, with a vertical scan from the surface to 90 km every 24.7 s. Each orbit consists of 240 scans spaced at 1.5° (165 km) along-track, with a total of almost 3500 profiles per day and latitudinal coverage from 82° S to  
20 82° N. The Level-1 limb radiance measurements are inverted using 2-D optimal estimation (Livesey et al., 2006) to produce Level-2 profiles of atmospheric temperature and composition. Validation of a previous version of the MLS H<sub>2</sub>O and HNO<sub>3</sub> data products and error estimations are discussed in detail by Read et al. (2007), Lambert et al. (2007) and Santee et al. (2007). MLS temperature validation and error analysis is discussed by Schwartz et al. (2008). Here we use the MLS version 4 (v4) data (Livesey et al., 2017), which have single-profile precisions (accuracies) of 4–15 % (4–7 %) for H<sub>2</sub>O, 0.6 ppbv  
25 (1–2 ppbv) for HNO<sub>3</sub> and for temperature a precision of 0.7 K and a bias in the range –2–0 K. We note that MERRA-2 assimilates MLS temperatures, but only at pressures less than 5 hPa and not within the pressure range investigated here (~~Bosilovich et al., 2015~~)(Gelaro et al., 2017).

Errors in the MLS H<sub>2</sub>O contribute a few tenths of a kelvin to the error in frost point temperature and are substantially smaller than the errors in the temperature limb sounding retrievals obtained from MLS. From August 2004 until December  
30 2013, mean differences between NOAA frost point hygrometer and MLS H<sub>2</sub>O (Hurst et al., 2014) showed no statistically significant differences (agreement to better than <1%) from 68–26 hPa, although significant biases at 100 and 83 hPa were found to be 10% and 2%, respectively. Increasing the time frame to mid-2015 (Hurst et al., 2016) suggests a long-term drift in MLS H<sub>2</sub>O of up to 1.5% per year starting around 2010. This is still under investigation by the MLS science team, but the

effect on the calculated STS reference and frost point temperatures would be less than 0.1 K per year. [Estimated uncertainties in the reference point temperatures are discussed in Sections 3.1 and 3.2.](#)

#### 2.4 [CALIPSO and Aura configuration within the A-train](#)

5 [CALIPSO and Aura are part of the afternoon “A-train” satellite constellation at 705 km nominal altitude and 98° inclination, with daily near-global coverage attained in 14.5 orbits. The initial A-train configuration of the CALIPSO and Aura spacecraft from April 2006 to April 2008 resulted in an across-track orbit offset of ~200 km, with the MLS tangent point leading the CALIOP nadir view by about 7.5 minutes. Since April 2008, Aura and CALIPSO have been operated to maintain positioning within tightly constrained control boxes, such that the MLS tangent point and the CALIOP nadir view are colocated to better than about 10-20 km and about 30 seconds.](#)

#### 10 2.5 COSMIC GPS RO temperatures

We use the US/Taiwan Constellation Observing System for Meteorology, Ionosphere and Climate (COSMIC) network data obtained from the Universities for Cooperative Atmospheric Research (UCAR) COSMIC Data Analysis and Archive Center (CDAAC). GPS RO data have provided high accuracy ( $< 0.2$  K, Gobiet et al., 2007), global (day and night) coverage, coupled with excellent long term stability for nearly two decades (Anthes, 2011). The introduction of GPS RO has been documented to  
15 improve NWP forecast skill in the ECMWF Integrated Forecast System (IFS) (Bonavita, 2014) and to reduce tropopause and lower stratospheric temperature biases in ERA-I (Poli et al., 2010). The direct assimilation of bending angles or refractivity is now the common practice for many global reanalyses; however, for many other purposes the production of vertical atmospheric temperature profiles from GPS RO data is required. Even though the RO measurements ~~per-seare SI-traceable of signal phase~~ [delays are traceable to the SI second](#) (Anthes, 2011), in common with all satellite limb sounding techniques, the retrieval of  
20 vertical atmospheric geophysical profiles from RO requires a number of assumptions because of the long ray path through a non-uniform atmosphere (Ho et al., 2012). Therefore, corrections are required for ionospheric effects, variations in water vapor, and gradients in temperature along the ray path (Poli and Joiner, 2004; Anthes, 2011). Many other studies have intercompared GPS RO with independent operational analyses, e.g. with forecast versions that have not assimilated the GPS RO data. The near real time COSMIC data (in the form of bending angles or refractivity) are ingested by most of the data assimilation procedures  
25 considered here (except for MERRA), and therefore these reanalyses are not strictly independent of the postprocessed COSMIC temperatures. We have chosen to use the COSMIC temperatures as a common reference to evaluate the reanalysis departures, rather than using the reanalysis ensemble mean.

[Schreiner et al. \(2007\) investigated the precision of the COSMIC data by leveraging the close configuration of the six satellites during the early deployment phase of the mission. Further work by](#) Staten and Reichler (2008) examined the tropopause  
30 temperatures obtained from various GPS RO datasets and determined a global mean bias of  $< 0.1$  K between the different RO instruments and of  $< 0.5$  K between RO instruments and radiosondes. A later study by the same authors (Staten and Reichler, 2009) reported a more comprehensive analysis of the RO temperature precision for the COSMIC data that examined variations with height, latitude and season. The concept of apparent precision was introduced, whereby the temperature differences

between colocated neighboring RO measurements are organized by their temporal and spatial differences. A quadratic polynomial surface was fit to the RMS temperature differences, acting as a noise filter for the atmospheric variability and providing the apparent temperature precision of perfectly colocated data via extrapolation of the fitted RMS values to the time and distance origin. For the 15 km to 26 km height range, the RMS differences increase monotonically from about 0.5 K to 1.5 K. The results presented graphically by Staten and Reichler (2009) appear to be applicable to the RMS of colocated measurement pairs and should therefore be divided by  $\sqrt{2}$  to represent the precision on a single GPS measurement.

Alexander et al. (2014) estimated the COSMIC GPS RO temperature precision by examining the RMS difference between a large ensemble of pairs of independent COSMIC observations (both wet and dry temperature profiles). Temperature accuracy was assessed by comparing to colocated ECMWF analyses, ~~and similar results were obtained over data sparse (Pacific) and data dense (USA) regions, with yielding~~ an average bias of 0.1 K (RO–ECMWF) for 10 to 30 km and  $-0.5$  K above 35 km. Comparisons of COSMIC GPS RO with ERA-I (Dee et al., 2011) showed deviations of  $\pm 1$  K at 100 hPa and  $\pm 2$  K at 10 hPa for the polar regions. Ladstädter et al. (2015) made COSMIC GPS RO comparisons to Vaisala RS90/92 radiosondes and found mean temperature differences for 100–30 hPa of  $<0.2$  K since 2006 and of  $<0.5$  K for 30–10 hPa. Scherllin-Pirscher et al. (2011b) modeled the observed vertical error structure of GPS RO measurements, including the dry temperature error variation. Differences between RO instruments from different missions were found to have global mean standard deviations differing by at most 0.2 K at all levels between 4 and 35 km. The GPS RO model error,  $s_{model}$ , is a constant value,  $s_0 = 0.7$  K around the tropopause, increasing exponentially with height into the stratosphere and given by

$$s_{model} = \begin{cases} s_0 & \text{for } z_{Ttop} < z < z_{Sbot}, \\ s_0 \exp\left[\frac{z - z_{Sbot}}{H_{Sbot}}\right] & \text{for } z_{Sbot} \leq z \end{cases} \quad (1)$$

where  $z_{Ttop}$  is the top level of the tropopause,  $z_{Sbot}$  is the bottom level of the stratopause. Latitudinal and seasonal variations are governed by an adjustable scale height parameter,  $H_S$ , which has its lowest values at high latitudes and during the winter months. The GPS model error has a different functional form for the troposphere (Scherllin-Pirscher et al., 2011b), which we do not require here.

The GPS RO data provide a measurement of the atmospheric refractivity,  $N$ , which is dependent on the temperature,  $T$  (in K), atmospheric pressure,  $p$  (in hPa), and the water vapor partial pressure,  $p_w$  (in hPa). For heights above 4 km, and following correction for ionospheric electron density,  $N$ , is given by (Smith and Weintraub, 1953)

$$N = c_1 \frac{p}{T} + c_2 \frac{p_w}{T^2} \quad (2)$$

where  $c_1 = 77.60$  K hPa $^{-1}$  and  $c_2 = 3.73 \times 10^5$  K $^2$  hPa $^{-1}$ . The first term in the equation represents the contribution to refractivity from the total molecular polarizability of the dry atmosphere, whereas the second term corresponds to the effects of the permanent dipole moment of water vapor molecules. In regions of low atmospheric humidity, above about 14 km at low latitudes and above about 9 km at high latitudes, dry temperatures provide an adequate representation of the physical atmosphere (Scherllin-Pirscher et al., 2011a). We used the latest available COSMIC GPS version 2013.3520 “atmPrf” dry temperatures processed at the UCAR CDAAC. These have been compared recently to Vaisala RS92 radiosonde temperatures

(Ho et al., 2017), and the mean radiosonde – RO global daytime temperature difference over 200–20 hPa was found to be 0.20 K, with a mean standard deviation of 1.5 K. For completeness, we also evaluated the “wetPrf” wet temperatures for the same data version from 2008 to 2013 in the polar regions. We obtained mean temperature differences (dry – wet) in the range –0.1 to +0.05 K at 100 hPa and –0.4 to +0.15 K at 10 hPa, with standard deviations of 0.15 K at 100 hPa increasing to 1.1 K at 10 hPa. The wet temperatures ~~are~~ yield results that are consistent with the dry temperatures and therefore are not considered further in this paper.

- 5 We have not implemented the line of sight corrections (Feltz et al., 2014b, a) that are possible when comparing against gridded temperature fields. On a case-by-case basis the correction can be  $>1$  K, depending on the orientation of the GPS raypath with respect to temperature gradients, but the raypath averaging method has been shown to reduce the bias (Feltz et al., 2014b, a). For larger sample sizes the biases are reduced because the positive/negative temperature gradients are averaged away even for a simple closest matching pair method (Feltz et al., 2014b, a).
- 10 ~~For convenience we interpolated (in log pressure) the COSMIC temperature profiles to a set of fixed pressure levels with 24 levels per decade ( $p = 1000 \times 10^{-i/24}$ ;  $i = 0, 49$ , approximately 2/3 km vertical resolution).~~ In Section 4.3 we compare each reanalysis data set to the COSMIC data and calculate the bias and standard deviation of the temperature differences.

### 3 Thermodynamics of PSC formation

The growth of solid nitric acid trihydrate (NAT) crystals is kinetically limited (e.g. Voigt et al., 2005) and is frequently out of  
15 equilibrium with the gas-phase  $\text{HNO}_3$  abundance. This makes NAT PSCs unsuitable for use as a local temperature reference, since their growth by  $\text{HNO}_3$  uptake is dependent on the temperature history (Larsen et al., 1997). On the other hand, liquid STS reacts more quickly to ambient temperature changes, effectively acting as a thermometer (Hoyle et al., 2013), provided that very rapid temperature changes are excluded (Voigt et al., 2005). Ice PSCs also react quickly to temperature changes, because of the high ambient  $\text{H}_2\text{O}$ . Critical supercooling is the temperature depression below the frost point where homogeneous freezing  
20 of the STS can take place to form ice (Larsen, 2000). A depression of about 3 K is typically required (Carslaw et al., 1998a; Koop et al., 1998). However, heterogeneous nucleation, such as the formation of ice on pre-existing NAT or freezing of STS mediated by active sites on foreign nuclei immersed within the liquid drop (Engel et al., 2013), does not require a temperature depression below the frost point.

Theoretical existence temperatures of the PSC types are calculated using equilibrium thermodynamics and are dependent on  
25 the ambient partial pressures of  $\text{H}_2\text{O}$  in the case of the ice frost point,  $T_{\text{ice}}$  (Murphy and Koop, 2005), and also  $\text{HNO}_3$  for STS (Carslaw et al., 1995). Errors in the calculations of these reference temperatures arising from uncertainties in the MLS  $\text{H}_2\text{O}$  and  $\text{HNO}_3$  data are estimated to be  $\leq 0.5$  K for  $T_{\text{ice}}$  and  $\leq 0.7$  K for  $T_{\text{eq}}$  in the pressure range 68–21 hPa.

It is expected that theoretical equilibrium calculations are more appropriate for ‘steady state’ conditions, e.g. PSCs produced by slow synoptic cooling, than rapidly changing temperatures associated with the cold phases of mountain waves  
30 ~~(Dörnbrack et al., 2001)~~ (Carslaw et al., 1998b; Dörnbrack et al., 2001). Therefore, mountain wave production of ice that is detected by the CALIOP wave-ice classification is excluded from this study. However, mountain wave activity also influences

the production of STS (Carslaw et al., 1998a). This can be potentially excluded to some extent by analysis of the wave activity in the reanalysis datasets (Knudsen, 2003) and rejection of data in the affected locations. Alternatively, since the CALIOP data have resolution superior to that of the reanalysis grids, we can address the challenge posed by the disparity between the CALIOP, MLS, and reanalysis horizontal and vertical sampling scales by selecting only those scenes with a consistent CALIOP PSC classification that fills a substantial proportion of the synoptic-scale MLS field of view (~~FOV~~) (see Section 4.4). Therefore, we can effectively mitigate the visual speckle effect (Pitts et al., 2009) of disparate PSCs occurring within the MLS field of view generated by sub-grid temperature fluctuations that are not resolved by the reanalysis data or that arise because of random noise in the CALIOP signals. Scenes satisfying this requirement for CALIOP STS detections we denote as LIQ, and for CALIOP ice detections we denote as ICE.

### 3.1 Ice cloud equilibrium

The frost point temperature (FPT,  $T_{ice}$ ) variation over the lower stratosphere is shown in Figure 1(a) for 5 ppmv  $H_2O$ . The FPT derivative, shown in Figure 1(b), indicates that a change in  $H_2O$  of 1 ppmv results in a change in FPT of  $\sim 1.05$ – $1.2$  K. The FPT derivative is used to convert the estimated MLS  $H_2O$  single-profile retrieval errors (Livesey et al., 2017) into an equivalent error in FPT, and the result is shown in Figure 1(c). The accuracy and precision are estimated to be 0.6–0.3 K and 0.3 K from 68–21 hPa, respectively. The root mean square error (RMS) is the quadrature addition of the accuracy and precision. Hence the estimated RMS errors in FPT arising from the uncertainties in the MLS  $H_2O$  measurements from 68–21 hPa are 0.7–0.4 K. As noted this is the error associated with a single measurement; although the statistical precision can be assumed to diminish as the square root of the number of measurements used for averaging, the accuracy remains as the overriding error source. In any case, the error in FPT is substantially lower than the estimated RMS errors for the MLS lower stratosphere temperature measurements (Section 2.3).

### 3.2 Supercooled ternary solution (STS) equilibrium

Sample STS equilibrium curves are calculated using the analytic formula of Carslaw et al. (1995) and shown in Figure 2(a) for a range of lower stratospheric conditions; pressures 68, 46, and 32 hPa;  $H_2O$  mixing ratios 4, 5, and 6 ppmv; and  $H_2SO_4$  mixing ratios 0.1 and 0.5 ppbv. Figure 2(b) shows the effect of removing the water vapor partial pressure variation through a coordinate transformation of the temperature scale relative to  $T_{ice}$ . In Figure 2(c) we show that the estimated accuracy and precision in  $T_{eq}$  arising from the uncertainties in the MLS  $HNO_3$  measurements from 68–21 hPa are 0.6–1.5 K and 0.4 K, respectively. The corresponding RMS errors are 0.7–1.6 K. This is greater than the FPT error, but still lower than the estimated RMS errors for the MLS lower stratosphere temperature measurements (Section 2.3).

## 4 Results

In order to provide context for the later results that use more complex analysis techniques, we first provide a basic overview of the reanalysis temperatures in the polar lower stratosphere, and we choose as a suitable metric the daily (12UT) mean 60°



30 polar cap temperature differences at 46 hPa for the 2008–2013 time frame. Figure 3 shows the timeseries of these temperature differences calculated for MERRA, MERRA-2, JRA55 and NCEP-CFSR relative to ERA-I, and smoothed using a 10-day boxcar average. Both hemispheres reveal underlying annual cycles with positive (negative) deviations in the summer (winter). In the Antarctic, MERRA displays the largest and most rapid excursions of up to 0.9 K from ERA-I, recurring in September through October every year, whereas in the Arctic the temperature excursions for all reanalyses are confined to within 0.5 K from ERA-I. The gray shaded regions in Figure 3 indicate the measurement periods we used for the main statistical analysis,  
 5 and although these were chosen in advance, based on capturing the bulk of the PSC formation, by chance they are synchronous with more stable plateau regions in the temperature differences for the Antarctic. Therefore to achieve valid comparisons with results from other investigations, one must first ascertain their compatibility based on their time overlap. We return to this theme in Section 4.5 concerning comparisons of the reanalyses with Antarctic measurements by superpressure balloons (Hoffmann et al., 2017a).

#### 10 4.1 Temperature fluctuations

Mesoscale temperature fluctuations have a significant effect on the formation of PSCs (Murphy and Gary, 1995; Dörnbrack and Leutbecher, 2001; Gary, 2006), and therefore the capability of models to accurately mimic PSC formation requires consideration of these sub-grid processes (Engel et al., 2014; Hoyle et al., 2013). The high vertical resolution of the COSMIC temperatures allows an examination of the spectrum of the temperature variance over the height region of PSC formation. For  
 15 this aspect of the analysis, we interpolated (in log pressure) the COSMIC temperature profiles to a set of fixed pressure levels with 24 levels per decade ( $p = 1000 \times 10^{-i/24}$ ,  $i = 0, \dots, 49$ , approximately 2/3 km vertical spacing). We have analysed the atmospheric temperature variability in the 80 to 20 hPa range by fitting cubic polynomials to the COSMIC profiles and calculating the mean variance,  $\overline{T'^2}$ , over this range. The cubic fit provides data smoothing to estimate the unperturbed background temperature state (Whiteway, 1999; Knudsen, 2003), and therefore the mean variance is a statistic that serves as a simple mea-  
 20 sure of the vertical wave disturbances. The orientation of the COSMIC line of sight to the planes of the gravity wave fronts (Preusse et al., 2002) has an influence on the detected wave amplitudes and hence the variances. No correction for this effect is attempted.

The mean temperature variance relative to the background unperturbed temperature state, i.e. the mean fractional variance  $\overline{\left(\frac{T'}{\bar{T}}\right)^2}$ , is related to the potential energy density of the wave disturbance,  $E_p$  in  $\text{J kg}^{-1}$ , by the relation (Whiteway, 1999; Tsuda  
 25 et al., 2000):

$$E_p = \frac{1}{2} \left(\frac{g}{N}\right)^2 \overline{\left(\frac{T'}{\bar{T}}\right)^2} \text{ J Kg}^{-1} \quad (3)$$

where  $g$  is the gravitational acceleration,  $T'$  is the perturbation amplitude,  $\bar{T}$  is the mean temperature, and  $N$  is the bouyancy frequency. Wave activity was categorized by Whiteway (1999) and Knudsen (2003) as inhibited for  $E_p < 1 \text{ J Kgkg}^{-1}$  and enhanced for  $E_p > 2 \text{ J Kgkg}^{-1}$ . Assuming typical values for the polar lower stratosphere,  $N \sim 0.02 \text{ s}^{-1}$ ,  $\bar{T} = 200 \text{ K}$ , we find  
 30 that an energy density of  $E_p = 1.5 \text{ J Kgkg}^{-1}$  corresponds to  $\overline{T'^2} = 0.5 \text{ K}^2$ , and we have used this value as a convenient variance threshold to delineate the transition between quiescent and enhanced wave activity.

The mean (2008–2013) [COSMIC vertical](#) temperature variances for the southern and northern ~~hemispheres~~ [hemisphere winters](#) are shown in Figure 4 for temperatures below 200 K. The Arctic temperature variance spectrum in Figure 4(d) shows a longer tail, extending well beyond  $1 \text{ K}^2$ , than for the Antarctic in Figure 4(a). The geographic distributions for the profiles with variances exceeding the  $0.5 \text{ K}^2$  threshold are shown in Figures 4(b,e). The signature of orographically forced gravity waves over the ~~Antaretic~~ [Palmer](#) Peninsula is captured by the variance statistic, even though it is not specifically tuned to detect orographic waves. Similarly, in the Arctic a slight increase in variance can be seen along the East coast of Greenland. These spatial imprints of gravity wave activity are largely consistent with the patterns identified by the AIRS  $15 \mu\text{m}$  brightness temperature variations ~~(?)~~ [\(Hoffmann et al., 2017b\)](#) and the ~~Antarctic winter monthly-mean~~ [Antarctic winter monthly-mean  \$E\_p\$  patterns also derived from COSMIC GPS-RO \(Hindley et al., 2015\)](#). However, since any kind of wave activity giving rise to vertical temperature fluctuations will increase the calculated variance, non-orographic features are also visible in these [COSMIC](#) temperature variance maps. Figures 4(a) and (d) indicate that around 4% and 12% of the COSMIC profiles exceed the  $0.5 \text{ K}^2$  ( $E_p = 1.5 \text{ J Kgkg}^{-1}$ ) threshold in the southern and northern hemispheres, respectively.

~~Small-scale temperature fluctuations cannot be captured accurately by the reanalysis data because of their limited spatial resolution. For example, a study of superpressure balloon measurements by Hoffmann et al. (2017a) found that ERA-I, MERRA and MERRA-2 reproduced about 30% of the standard deviation of the balloon temperature fluctuations, whereas the lower spatial resolution NCEP/NCAR reanalysis reproduced only 15% and the higher resolution ECMWF operational analysis reproduced 60%. ECMWF analyses also underestimate both gravity wave momentum fluxes derived from the balloon measurements (Jewtoukoff et al., 2015) and wave amplitudes derived from Aqua AIRS (Hoffmann et al., 2017b). Similarly, the COSMIC data should perform better than the reanalyses because of their higher resolution.~~ The standard deviation of the differences between the reanalysis and COSMIC temperatures is the result of the quadrature addition of their [individual](#) standard deviations. ~~Small-scale temperature fluctuations cannot be captured accurately by the reanalysis data, but the COSMIC data should perform better because of their higher vertical resolution. A decrease in the spread of~~ [The effect of removing the colocated profiles that show gravity wave activity should be to decrease the spread in the](#) temperature differences of reanalysis data compared to COSMIC ~~should be detectable by rejecting the temperature profiles from consideration that are expected to have lower fidelity to the true atmosphere.~~ This is seen to be the case in Figures 4(c) and (f), where the standard deviations of the temperature differences between ERA-I and COSMIC improve successively as the more highly fluctuating profiles (as determined by the COSMIC mean [vertical](#) temperature variances) that are less well captured by the ERA-I reanalysis scheme are excluded.

The mean differences are also seen to improve substantially for the Arctic, but not for the Antarctic. Another effect to consider is that this method also reduces the variability of the atmospheric path along the COSMIC line of sight, and consequently the fidelity of the COSMIC temperatures to the true atmosphere will also be improved. Therefore, we cannot attribute the entirety of the observed reduction in the standard deviation to the ERA-I reanalysis data alone.

~~In the~~ [We have analyzed the other reanalyses with respect to the mean and standard deviations from the COSMIC temperatures, also using the COSMIC estimate of  \$E\_p\$  as an effective means of applying low-pass filtering to reveal the large-scale temperature structure as described above for ERA-I. Similar to the results in Figures 4\(c\) and \(f\) for ERA-I, we also find smaller standard deviations for the other reanalyses for the low-pass filtering cases \(not shown\).](#)

~~In the main statistical analysis of the large-scale~~ reanalysis temperature comparisons with COSMIC ~~in Section ?? we have excluded we have applied a low-pass filter by excluding~~ profile matches with COSMIC temperature variance  $>0.5 \text{ K}^2$  ( $E_p > 1.5 \text{ J K g kg}^{-1}$ ), ~~and~~. We have also restricted the COSMIC temperatures to below 200 K to better match the regions of potential PSC formation.

## 4.2 Orographic gravity wave case study

In the next section we report on the statistical analysis of the temperature differences, but first we examine a case study taken from a synoptic cooling period coupled with a gravity wave event on 28 August 2008 (2008d241) over the ~~Antaretic~~ Palmer Peninsula region as shown in Figure 5. The ~~case study serves to illustrate the quite large differences in the representation of wave structure between the reanalyses and the dependence on the spatial resolution.~~ The 50 hPa maps (Figure 5(a)) show the reanalysis temperatures at 18UT on 28 August 2008, and a large variation in the wave activity is seen, with JRA-55, ERA-I and NCEP having much larger amplitudes than GEOS-5.9.1, MERRA and MERRA-2. A longitude section from  $-70^\circ$  to  $-50^\circ$  at latitude  $72^\circ \text{ S}$  is selected for further study. The mountain wave is forced by flow over the topographic ridge along the ~~Antaretic peninsula~~ Palmer Peninsula, and the wind direction is almost orthogonal to the ridge line, with wind speeds  $u \sim 25\text{--}35 \text{ ms}^{-1}$  ~~corresponding to the observation of ice clouds in the pressure range 80–40 hPa~~. The vertical wavelength,  $\lambda_z$ , is about 7–8 km, with a temperature amplitude of  $\pm 12 \text{ K}$  determined by MLS. PSC ice formation detected by CALIOP (not shown) correlates with the cold phases of the gravity wave, but not with all regions colder than the frost point. The horizontal wavelength,  $\lambda_h \sim 400\text{--}500 \text{ km}$ , is resolved by AIRS (not shown) using the techniques of Eckermann et al. (2009). From the linear gravity wave dispersion relation, we obtain the vertical wavelength,  $\lambda_z = 2\pi u/N$ , in the range 7–11 km, in agreement with that observed.

Figure 5b shows the temperature variation at five pressure levels (100, 70, 50, 30 and 20 hPa) along the longitude section. Temperatures below the ice frost point, calculated using MLS  $\text{H}_2\text{O}$ , are highlighted by square symbols, and the mountain terrain is indicated by the black shading. At 50 hPa the peak to trough temperature differences are 7.4, 6.2, 8.0, 10.0, 6.1 and 14.9 K for GEOS-5.9.1, MERRA, MERRA-2, JRA-55, ERA-I and NCEP-CFSR, respectively; i.e., over a factor of two difference is seen in the temperature amplitudes between the reanalyses. ~~These differences in the wave amplitudes are rather well correlated with the spatial resolutions of the reanalyses (see Table 1).~~ Figures 5(c) and (d) show the time variation of the gravity wave induced temperature disturbance during 28–29 August, along the longitude section at 50 hPa and 30 hPa, respectively. It is clear from these figures that the height variation, timing of the onset and extent of temperatures cold enough to potentially form ice PSCs are quite different in each of the reanalyses. The lowest temperatures are below the ice frost point at every time stamp for the 30-hPa NCEP-CFSR data, whereas for ERA-I the temperatures are only sporadically below the ice frost point. In this particular case, a PSC model run based on the NCEP-CFSR temperatures would clearly produce much larger, and longer lasting, ice volumes than one using the ERA-I temperatures.

~~In the rest of this paper we concentrate on the large-scale temperatures, facilitated by the effective low-pass filtering using the  $E_p$  threshold to remove gravity-wave fluctuations. However, further work on issues related to the representation of gravity waves in the reanalyses would be worthwhile, and the high-pass side of the  $E_p$  threshold may provide useful insights.~~

#### 4.3 Reanalysis ~~temperature difference distributions~~ temperatures compared to COSMIC, ~~$T_{re} - T_{ro}$~~ GPS RO

Distributions of the temperature differences between the reanalyses and COSMIC were compiled for the polar regions for the 100–10 hPa pressure range. The ~~geophysical~~ structure of the temperature differences has been obtained from summary statistics consisting of zonal medians and standard deviations calculated over the 2008–2013 period (Figure 6). Both JRA-55 and NCEP-CFSR show abrupt vertical transitions in the median differences above 21 hPa in both hemispheres. This is likely to be an interpolation error in the case of NCEP-CFSR since the 14.7 hPa common vertical grid level is distant from the closest native vertical grid points at 20 and 10 hPa. However, for JRA-55 the native vertical grid has a higher vertical resolution and the interpolation error is small. The standard deviations for the Arctic are similar in zonal structure for all the reanalyses, but the values are systematically smaller in the Antarctic.

Figure 7 is a summary of the temperature bias ranges, extracted from the data shown in Figure 6, that readily captures the salient information over the pressure range from 68 to 21 hPa, which encompasses the bulk of the PSC vertical formation region (Pitts et al., 2009). The main attributes of the reanalyses are revealed by the relative size of the boxes and their location relative to the zero line. The box width is set to the largest difference in minimum to maximum bias at any height (68–21 hPa), and the box height is set to the largest difference in minimum to maximum meridional bias. The MERRA boxes are larger than those for any of the other reanalyses, with widths (heights) of 0.54 K (0.54 K) in the Antarctic and 0.86 K (0.50 K) in the Arctic. The smallest box widths are for Arctic NCEP-CFSR (0.26 K) and Antarctic JRA-55 (0.26 K). The smallest box heights are for Arctic NCEP-CFSR (0.18 K) and Antarctic MERRA-2 (0.14 K).

For both polar regions the reanalysis temperature differences from COSMIC are encompassed within a quite narrow range of  $-0.61$  to  $+0.48$  K. GEOS-5.9.1, MERRA, MERRA-2 and JRA-55 have cold biases ( $-0.61$  to  $-0.05$  K) in the Antarctic, whereas ERA-I has a warm bias ( $+0.04$  to  $+0.38$  K). The NCEP-CFSR bias ( $-0.30$  to  $+0.16$  K) changes with decreasing pressure from warm to cold. Overall, the average Arctic temperature biases for individual reanalyses with respect to COSMIC are shifted by  $\sim 0.1$ – $0.4$  K from the Antarctic values.

#### 4.4 ~~Relative proportion of CALIOP PSC types~~ within from CALIOP and their representation in MLS ~~FOV~~ observations ~~geometric~~

Figure 8 is an example of the probability density distribution, presented as a ternary graph, of the relative proportion of the three groups of CALIOP PSC types, STS, MIX and ICE occurring within the MLS geometric field of view. Here we define the congener names MIX, for the sum of the MIX1, MIX2, and MIX2-enh types, and ICE, which also includes wave-ice. This figure is compiled by accumulating the co-existence frequency of these three groups of PSCs for the 2013 Antarctic winter on the 46 hPa pressure level for temperatures below the ice frost point (as determined by ERA-I). The three axes lie along the sides of an equilateral triangle, and the three components are constrained to sum to unity. At the center of any side the percentage of the two adjoining PSC types is 50:50, and the third type at the opposite vertex is zero. At the center of the triangle the proportion of all three PSC types is equal to  $1/3$ . The most populated areas consist of two branches close to the MIX/STS and MIX/ICE axes. Away from these two branches, the STS/ICE region with less than 10% MIX is essentially devoid of data.

This graph is a striking demonstration that the co-existence of STS and ice PSCs on a spatial scale of the size of the MLS geometric field of view is relatively rare. The implication is that the rapidity of freezing of STS to form ice and the resulting re-equilibration of the water vapor and cloud ice is faster than can be captured by the satellite instrument integration times. The A-train orbital speed is  $\sim 7.5 \text{ km s}^{-1}$ , and hence the 165 km along-track MLS FOV is traversed in about 22 s.

#### 4.5 ~~MLS field-of-view PSC fill-fraction~~

We illustrate the concept of the field of view fill-fraction in Figures 9 ~~and~~ 10. Figure 9 shows CALIOP and MLS data recorded over a 7000 km transect over Antarctica on 23 June 2008 (2008d175). The CALIOP PSC types show large contiguous areas of STS and ice, but with other embedded PSC types causing visual speckle as mentioned above (Figure 9(a)). The MLS temperatures are up to 4 K below the frost point (Figure 9(b)). Large regions of  $\text{HNO}_3$  depletion are seen where abundances have been reduced to practically zero values by sequestration and denitrification by PSCs compared to background values of over 12 ppbv (Figure 9(c)). A smaller dehydrated region has  $\text{H}_2\text{O}$  values 1-2 ppmv lower than the  $\sim 5$  ppmv background (Figure 9(d)). The second and third rows in the figure show expanded views of a selected region at 32 hPa centered on a particular MLS geometric field of view. At each magnification step the CALIOP data reveal increasingly finer detail down to the 5-km by 0.180 km pixel size, whereas the MLS data become over-sampled.

~~Figure ?? shows the corresponding CALIOP PSC types and the Feature Mask information within the~~ Within the highlighted ~~MLS geometric field of view shown in Figure 9. The CALIOP feature mask is a 3-digit number, N1N2N3, where N1 encodes~~ information on the height of each “pixel” relative to the local tropopause (Figure ??(b)) and N2N3 encodes information on the ~~horizontal averaging (5 to 135 km) and the backscatter threshold used for detection (Figure ??(e)). In this particular case, all~~ pixels are at least 4 km above the tropopause, and the majority of pixels are detected with a horizontal averaging of 45 km or ~~smaller.~~

~~The fraction of the MLS FOV occupied by the different PSC types (Figure ??(a)) is calculated and given in the figure~~ caption, all CALIOP PSC types except wave ice are present, consisting of STS:68.9%, ICE:1.6%, MIX1:0.6%, MIX2:12.9%, ~~and MIX2E:13.2%. Clear sky cases make up the remaining 2.8%.~~ We impose an upper limit on the occupancy fraction of cloud-free pixels of 0.25 and require the fraction of the dominant LIQ or ICE PSCs to be greater than 0.75. The example scene has too great a variation of PSC types within the MLS field of view and fails this acceptance test since it only has a 0.69 LIQ fill-fraction. Orbit transects of the MLS FOV PSC fill-fraction for the different PSC types are shown in Figure 10. The LIQ and ICE filled FOV threshold criteria are mutually exclusive. Despite the PSCs extending over a few thousand km, the strict acceptance criteria, albeit essential to ensure a more uniform single PSC type across the MLS FOV, severely reduces the total number of scenes available for analysis. Only about 15% of the scenes containing STS or ice PSCs are accepted.

#### 4.5 ~~Reanalysis temperatures compared to LIQ and ICE reference points~~

~~We select viewing scenes in which there is a distinct dominant PSC classification in a sample volume that is similar in size to~~ the MLS gas species resolution. As discussed above the requirement is that 75% or more of the CALIOP pixels in the MLS ~~geometric FOV have the same PSC classification.~~

~~We summarize the method below:-~~

~~Identify LIQ and ICE PSCs using the CALIOP lidar measurements. Accumulate the CALIOP PSC types (LIQ and ICE) at the MLS along-track resolution (165 km  $\times$  2.16 km), ensuring that the same PSC type is detected in at least 75% of the MLS field of view. Calculate the theoretical temperature dependence of STS ( $T_{eq}$ ) and ice ( $T_{ice}$ ) PSCs under equilibrium conditions using the spatially and temporally collocated MLS gas-phase and measurements. Compare (a) calculated and observed uptake in STS and (b) ice temperature distribution vs frost point with reanalysis data and MLS temperatures. Create LIQ and ICE temperature distributions for each data set: GEOS-5.9.1, MERRA, MERRA-2, JRA-55, ERA-I, NCEP-CFSR (all sampled by interpolating to the MLS measurement times and locations) and MLS temperature. Calculate median and mean temperature deviations from  $T_{eq}$  and  $T_{ice}$  and their standard deviations for LIQ and ICE classifications, respectively.~~

#### 4.5 Distributions of observed MLS and theoretical equilibrium and gas-phase variation with temperature

10 Figure 11 shows scatter plots of the coincident MLS  $\text{HNO}_3$  and  $\text{H}_2\text{O}$  for Antarctic PSCs classified by CALIOP vs ERA-I temperature at 46 hPa in 2013. Figures 11(a) and (c) show the scatter of  $\text{HNO}_3$  vs temperature and inverse temperature, respectively, along with the theoretical  $\text{HNO}_3$  gas-phase uptake curves for STS and NAT, indicating clearly that LIQ PSCs are closely associated with the STS curve. Similarly, Figures 11(b) and (d) show the scatter of gas-phase  $\text{H}_2\text{O}$  and its close association with the frost point temperature in the presence of ICE PSCs.

15 In Figure 12 we show the temperature variation of the estimated partial pressure of water vapor over ice,  $p_{ice}$ , for atmospheric pressure levels in the range 100–10 hPa. The partial pressure is determined simply from the product of the MLS  $\text{H}_2\text{O}$  volume mixing ratio and the atmospheric pressure. Since CALIOP indicates the presence of coincident ice PSCs, this is an estimate of the partial pressure of water vapor over ice. The bias in the MLS temperatures is evident in the departure of the  $p_{ice}$  observations from the theoretical equilibrium curve in Figure 12(a), whereas the ERA-I temperatures place the  $p_{ice}$  observations in much  
20 better agreement.

#### 4.5 Polar temperature Reanalysis temperatures compared to LIQ and ICE reference points

In Figure 13 we show the variation of the MLS gas-phase  $\text{HNO}_3$  with ERA-I temperature corresponding to CALIOP PSC classifications at 32 hPa for one Southern Hemisphere winter. The MLS  $\text{HNO}_3$  data are separated into corresponding CALIOP PSC categories, allowing comparison of observed and modeled uptake of  $\text{HNO}_3$  in different types of PSCs. The scatter of MLS  
25  $\text{HNO}_3$  against the temperature deviation from the frost point (calculated using MLS  $\text{H}_2\text{O}$ ) is shown in Figure 13(a) for LIQ and ICE PSCs. The  $\text{HNO}_3$  gas-phase uptake in the presence of liquid-phase LIQ PSCs follows the STS equilibrium curve. In contrast, the  $\text{HNO}_3$  abundance is very low in the presence of ICE PSCs. In Figure 13(b), the  $\text{HNO}_3$  gas-phase uptake in clouds associated with the CALIOP solid NAT type MIX2 shows significant non-equilibrium variation and lies between the STS and NAT equilibrium curves. Histograms of the temperature distributions of (a) and (b) are shown in Figure 13(c). The light blue  
30 (LIQ) and yellow (MIX2) colored histograms are for  $\text{HNO}_3$  mixing ratios  $>1$  ppbv, whereas the red (LIQ) colored histogram is for  $\text{HNO}_3$  mixing ratios  $<1$  ppbv. The tails of the temperature distributions for LIQ (light blue and red histograms) do not extend to temperatures lower than those in the distribution for ICE (dark blue), and no peaks are observed that would



indicate the existence of PSCs at a frost-point depression near  $T_{\text{ice}} - 3$  K. In Figure 13(d), the temperatures are transformed according to the STS equilibrium curve for the LIQ classification and NAT equilibrium curve for the MIX2 classification; the ICE classification remains the same as in (c) for comparison. Note that the LIQ histogram is shifted and becomes much narrower (Lambert et al., 2012). This is just an illustrative case; since there are seven temperature data sources, collected over 5 six years on six pressure levels, the total number of histograms is ~~252~~252 for each hemisphere.

#### 4.5.1 **Statistics of the temperature difference distributions, $T_{\text{re}} - T_{\text{eq}}$ , for each reanalysis and comparison to the normal distribution**

Statistics for each reanalysis data set of the temperature difference distributions were generated from histograms analogous to those in Figure 13(d) for each year and pressure level. ~~The~~Statistics of the combined data for the 2008–2013 Antarctic 10 winters at 46 hPa are ~~displayed in Figure ?? for the LIQ PSCs and Figure ?? for the ICE PSCs~~shown in Tables 2 and 3. The distributions for LIQ PSCs (Table 2) all show negative temperature biases compared to the STS equilibrium reference, with mean values in the range  $-0.9$  to  $-0.3$  K and standard deviations  $\sim 0.6$  K. The standard error of the mean is  $\sim 0.01$  K, and the medians are very similar to the mean values, indicating a small skewness of the distribution. ~~Visually, the~~The scatter follows a normal distribution reasonably well in the tails of the distribution, but with a mismatch near the peak of the distribution 15 (not shown). The normalized  $\chi^2$  values are in the range 1.4–2.2, which for around 30 degrees of freedom (i.e. the difference between the number of histogram bins and the number of fitted parameters) indicates a poor goodness-of-fit. We note that improved fits can be obtained by introducing a secondary normal distribution with a smaller standard deviation (not shown), which seems to imply the underlying presence of two distinct modes of temperature precision in the reanalyses. We have not 20 investigated this finding any further, but one pertinent avenue of exploration, given that the density of observations ingested into the system is sparse in the polar regions, would be to look for evidence that the reanalysis temperatures near grid points that are located closer to the geographic source of assimilated observations have better precision than those at grid points remote from observations.

The distributions for ICE PSCs (Table 3) show mainly negative temperature biases compared to the equilibrium ice frost point reference. Mean temperature bias values for ICE PSCs are in the range  $-0.6$  to  $0$  K with standard deviations of  $\sim 0.7$  K, 25 both of which are larger than their LIQ PSC counterparts. The ICE distribution fits were also improved in some cases by introducing a secondary normal distribution.

#### 4.5.1 **Reanalysis temperature difference distributions compared to the LIQ and ICE references, $T_{\text{re}} - T_{\text{eq}}$ , and COSMIC GPS RO, $T_{\text{re}} - T_{\text{ro}}$**

Intercomparisons of the reanalysis temperature ~~distributions derived from the data in Figures ?? and ??~~statistics are displayed 30 in Figure 14 for the Antarctic in 2013 (a representative year). In addition to the differences relative to the LIQ and ICE reference points, we also show the comparison with the COSMIC temperatures (latitude range  $90^\circ$  S to  $60^\circ$  S, mean variance  $< 0.5$  K<sup>2</sup> and COSMIC temperatures  $< 200$  K). The largest bias is for MLS, and biases for the LIQ reference are consistently about  $0.5$  K more negative than for ICE. Biases for the COSMIC reference are smaller than those for LIQ or ICE. MERRA



does not assimilate the COSMIC GPS RO data, and it has the largest bias with respect to the COSMIC reference. Standard deviations for LIQ are consistently smaller than those for ICE, and standard deviations for COSMIC are between those of LIQ and ICE. Interannual variability for the 46 hPa level is shown in Figure 15, where median values for the COSMIC reference display less variability than those for the LIQ or ICE references. Two years (2010 and 2012) stand out in the LIQ median reference as anomalously high, and we note that those Antarctic winters were warmer than in the other years (Kuttippurath et al., 2015). Standard deviations show less interannual variability than median values, especially for the COSMIC reference.

The vertical temperature differences over the 100–10 hPa range are shown in Figure 16 for the Antarctic winters 2008–2013. Median values for the ICE reference are more constant with height than those for the LIQ reference, which become more negative with increasing height. Median values for the LIQ reference are biased lower than those for ICE by  $\sim 0.5$  K, although standard deviations for the LIQ reference are smaller than those for ICE. The corresponding observations for the Arctic are shown in Figure 17, but there the number of data points in the ICE reference is much lower, [and the lack of sufficient ice cloud production in the Arctic precludes a robust conclusion for ICE PSCs](#). Again, MLS shows the largest bias.

Das and Pan (2014) intercompared COSMIC GPS RO temperatures with satellite measurements from the Sounding of the Atmosphere using Broadband Emission Radiometry (SABER) instrument and Aura MLS and determined that the structure of the observed median temperature differences was due in large part to inherent retrieval biases of SABER and MLS (December 2010 to November 2011). Seasonal and meridional bins were used to compare with SABER and MLS. At high latitudes, in the 100–10 hPa range, median profiles for SABER showed an obvious positive bias (2–3 K higher than COSMIC) in the lower stratosphere, increasing with decreasing atmospheric pressure. Median profiles for MLS showed negative biases of 0 to 2 K, but with larger oscillations than seen with SABER. These results indicate the difficulty of obtaining sub-kelvin temperature accuracy with microwave and infrared limb sounders.

The standard deviations result from the combination of the quadrature addition of the precisions of the reanalyses and the reference points. In Figures 1 and 2, we estimated the minimum precision of the ICE and LIQ references to be  $\sim 0.3$  K. For the LIQ reference comparison (Figures 16(d) and 17(d)), the minimum combined precision is 0.5 K (in both NH and SH); therefore, subtracting the LIQ reference precision results in an estimated precision of 0.4 K for the reanalysis data. The theoretical vertical structure of the COSMIC GPS RO standard deviation values follows an exponential increase with height as shown by Scherllin-Pirscher et al. (2011b) and is defined by Equation 1. We have determined the best fit parameters for each hemisphere from Equation 1 by minimizing the RMS deviations of the ensemble means of the (reanalysis – COSMIC) standard deviations. The solid black lines in Figures 16(f) and 17(f) are the quadrature addition of the estimated reanalysis temperature error,  $\sigma_{T_{RE}} = 0.4$  K, and the GPS RO model error given in Equation 1 with best fit parameters  $s_0 = (0.83, 0.69)$  K,  $H_s = (10.1, 8.8)$  km, and  $Z_s = (22.5, 23.1)$  km for the Arctic and Antarctic, respectively; i.e. our values for  $s_0$  are close to the 0.7 K value given by Scherllin-Pirscher et al. (2011b).

The MERRA temperatures should be uncorrelated with the COSMIC data, and in the main they do show a higher combined standard deviation than the other reanalyses. Some correlation with the other reanalyses that assimilate COSMIC data may be expected to reduce the standard deviation, and this appears to be the case except for the top two pressure levels.

35 For the southern hemisphere, the LIQ reanalysis standard deviation (Figure 16(d)) appears to be approximately constant from 46 to 14 hPa, rising at the lower stratospheric levels, whereas the northern hemisphere (Figure 17(d)) shows no increase at the lower levels. Overall the combined standard deviations for the reanalyses and COSMIC data are higher in the Arctic (Figure 17(f)) than in the Antarctic (Figure 16(f)) by  $\sim 0.1$  K.

5 Recently, Hoffmann et al. (2017a) used superpressure balloon measurements made during the Antarctic Concordiasi campaign in September 2010 to January 2011 to validate meteorological analyses and reanalyses. Over the flight paths of the balloons (17–18.5 km (58.2–69.1 hPa) and 60° S – 85° S), Hoffmann et al. found warm biases ranging from 0.6 to 1.5 K for ERA-I, MERRA and MERRA-2, increasing towards the pole, and standard deviations of 0.5–0.8 K, with ERA-I showing smaller standard deviations than MERRA. Whereas Hoffmann et al. find MERRA to be the warmest and ERA-I the coldest, we find the opposite order compared to the COSMIC and thermodynamic temperature references (see Figure 16). Also we  
10 find negative temperature biases for MERRA and MERRA-2 and only a slight positive bias for ERA-I, with no significant latitudinal gradients (Figure 6). To reconcile this apparent discrepancy we show daily mean temperatures (at 12UT) for MERRA and MERRA-2 relative to ERA-I in Figure 18 and highlight the non-overlapping time periods of the PSC analysis window (green line) and the balloon flights (red line). Clearly, measurements in the later time period of the balloon flights (September–December) sample different atmospheric conditions than experienced in the earlier time period (May–August).  
15 Differences between reanalysis temperatures along the individual balloon trajectories are likely to be amplified compared to the differences in mean polar cap temperatures.

As we noted previously MERRA does not assimilate COSMIC data, whereas MERRA-2 and the other reanalyses we investigated do assimilate COSMIC data, and hence some of the reduction in the bias of MERRA-2 compared to MERRA seen in Figure 18 is likely to be attributable to the use of GPS RO data in the former.

20 Large vertical oscillations of up to  $\pm 2$ –3 K were reported in the differences between ECMWF operational analyses and the CHallenging Minisatellite Payload (CHAMP) RO data in the 2002 to 2006 June–August Antarctic polar vortices (Gobiet et al., 2005, 2007). Similar height-dependent features were also found (Parrondo et al., 2007) in comparisons of ECMWF analyses with radiosondes. The value of the RO dataset as a reference was ably demonstrated by comparisons of CHAMP RO with ECMWF and other meteorological data (GEOS-4, MetO, NCEP/CPC, NCEP Rean) for June–August 2003 (Gobiet et al., 2007). None of the  
25 other dataset differences showed features consistent with ECMWF, nor were any two consistent with each other, e.g. GEOS-4 displayed an Antarctic cold bias relative to CHAMP at 25–30 km, whereas NCEP Rean displayed a warm bias in roughly the same range. The absence of spurious vertical features in the comparisons we have presented here underlines the general much closer agreement amongst the more modern reanalysis systems.

Although we have not directly matched A-train locations with the COSMIC occultations, we can estimate the differences be-  
30 tween the COSMIC temperatures and the thermodynamic reference temperatures by elimination of the reanalysis temperature biases as follows. First, we decompose the reanalysis, radio occultation and equilibrium temperatures into  $T_x = T' + \Delta T_x$ , where  $T'$  is the true temperature, and the temperature bias is  $\Delta T_x$ , such that  $x = \text{re, ro, eq}$  for the reanalysis, radio occultation and equilibria, respectively. Then, we have  $\overline{(T_{\text{re}} - T_{\text{ro}})} = \overline{\Delta T_{\text{re}}} - \overline{\Delta T_{\text{ro}}}$  and  $\overline{(T_{\text{re}} - T_{\text{eq}})} = \overline{\Delta T_{\text{re}}} - \overline{\Delta T_{\text{eq}}}$ . With the tacit implication that the  $\overline{\Delta T_{\text{re}}}$  are unchanging and can be eliminated from both equations, we derive  $\overline{(T_{\text{re}} - T_{\text{eq}})} - \overline{(T_{\text{re}} - T_{\text{ro}})} =$

$\overline{\Delta T_{ro}} - \overline{\Delta T_{eq}}$ . The results of these operations are shown in Figure 19 for LIQ and COSMIC,  $\overline{\Delta T_{LIQ}} - \overline{\Delta T_{COSMIC}}$ , and ICE and COSMIC,  $\overline{\Delta T_{ICE}} - \overline{\Delta T_{COSMIC}}$ . The temperature bias difference profiles for the different reanalyses are very closely grouped, especially over the pressure range 68–21 hPa, justifying the assumption that  $\overline{\Delta T_{re}}$  can be eliminated. The biases for  $(\overline{\Delta T_{LIQ}} - \overline{\Delta T_{COSMIC}})$  are similar in their shape and value for both hemispheres over the pressure range 68–21 hPa, with  $\overline{\Delta T_{LIQ}}$  around 0.5 to 1.0 K lower than  $\overline{\Delta T_{COSMIC}}$ . The biases for  $\overline{\Delta T_{ICE}}$  are around 0 to 0.5 K lower than  $\overline{\Delta T_{COSMIC}}$  for the Antarctic, but the Arctic has too few data points to make a meaningful comparison. The LIQ and ICE profiles for the Antarctic have similar values at 32 hPa with  $\overline{\Delta T_{ICE}} - \overline{\Delta T_{COSMIC}} \sim -0.5$  K, whereas the LIQ values diverge from those of ICE by up to  $-1.5$  K above and below this level. The reasons for these LIQ and ICE systematic discrepancies are not known; however, the differences are within the expected uncertainty limits in the 68–21 hPa pressure range.

Finally, a summary of the mean temperature bias ranges of the reanalyses relative to the LIQ ( $-1.6$  to  $-0.3$  K) and ICE ( $-0.9$  to  $+0.1$  K) equilibrium references and COSMIC ( $-0.5$  to  $+0.2$  K) is shown in Figure 20. The ranges quoted are for the pressure range 68–21 hPa. For all reference points, the coldest reanalysis biases tend to be found in the Antarctic and the warmest in the Arctic.

## 5 Conclusions

We have evaluated the accuracy and precision of several contemporary reanalysis data sets compared to (a) the COSMIC GPS RO temperatures and (b) the absolute temperature references obtained from the equilibrium properties of certain types of PSC. In the polar regions, for temperatures below 200 K, the range in the mean biases of the reanalyses with respect to COSMIC temperatures is only  $-0.61$  to  $+0.48$  K. The lack of assimilated GPS RO data in MERRA is more evident in the higher biases for this data set with respect to COSMIC temperatures in the Antarctic (i.e. where there is a relative paucity of conventional measurements) compared to the other reanalyses. Significantly larger negative biases, except at 100 hPa, and a vertical oscillation are seen in the MLS temperatures. Standard deviations are similar for the reanalyses, but the standard deviations for MLS temperature are substantially larger.

The extent to which the equilibrium thermodynamics of STS and ice PSCs can be used as absolute temperature references has been explored in detail. The estimated measurement precisions for the STS equilibrium and ice frost points are 0.4 K and 0.3 K, respectively, in the 68–21 hPa pressure range. The corresponding estimated measurement accuracies are in the range 0.7–1.6 K for STS and 0.4–0.7 K for ice. The resulting RMS uncertainties are smaller than those derived for the MLS retrieved temperatures and comparable to the measurement capabilities of the GPS RO technique (accuracy  $< 0.2$  K, precision  $> 0.7$  K) in the lower stratosphere. The reanalysis temperatures were found to be lower than the absolute reference points by 0.3 to 1 K for LIQ and 0 to 1 K for ICE at the peak heights of PSC occurrence (68–32 hPa). Vertical profiles for LIQ show larger negative deviations above 32 hPa than below that level, and also compared to ICE. Medians for LIQ are consistently biased lower than those for ICE by  $\sim 0.5$  K. On the 46 hPa pressure level, medians of the reanalyses all depart from zero, and their scatter falls within the range of about 0.6 K for LIQ and 0.5 K for ICE. Although the biases are larger for LIQ than for ICE, the standard deviations for LIQ ( $\sim 0.6$  K) are smaller than those for ICE ( $\sim 0.7$  K).

To put these LIQ and ICE reference temperatures into context with other independent polar temperature measurements, it is instructive to compare them to the temperature measurement errors from long-duration balloon flights, which have typical nighttime biases of 0.5 K, precisions of 0.4 K (Pommereau et al., 2002) and measured standard deviations of 1.0 to 1.3 K for temperature differences with respect to ECMWF operational analyses (Knudsen et al., 2002).

The polar temperatures from several contemporary reanalyses are in much better agreement than were the reanalyses from previous decades. Hence, in explaining any systematic deficiencies in modeled chlorine activation and/or modeled ozone losses based on these reanalyses, the burden shifts to finding alternative explanations other than the arbitrary adjustment of the reanalysis temperatures by as much as 1–2 K to offset such discrepancies. However, even though the reanalysis temperature differences are in general in very good agreement, under certain conditions such as wave-driven events, individual temperature comparisons may vary by several kelvin and are therefore important for specific case studies.

## 6 Data availability

MLS data are archived at the NASA Goddard Earth Sciences Data Information and Services Center (Schwartz et al., 2015; Lambert et al., 2015; Manney et al., 2015).

CALIOP data were obtained from the NASA Langley Research Center Atmospheric Science Data Center (CALIOP L1; CALIOP L2).

COSMIC data were obtained from the University Corporation for Atmospheric Research COSMIC Data Analysis and Archive Center (COSMIC)

GEOS5.9.1 data were obtained from the Goddard Earth Sciences Data and Information Services Center (GEOS5.9.1).

MERRA data were obtained from the Goddard Earth Sciences Data and Information Services Center (MERRA).

MERRA-2 data were obtained from the Goddard Earth Sciences Data and Information Services Center (MERRA2).

JRA-55 data were obtained from the Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory JRA-55.

~~ERA-Interim~~ ERA-I data were obtained from the Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory (ECMWF)

NCEP-CFSR data were obtained from the Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory (NCEP-CFSR).

IDL software for calculation of PSC thermodynamic properties provided by M. E. Hervig was obtained from the GATS Scientific Software 95 website ([http://gwest.gats-inc.com/software/software\\_page.html](http://gwest.gats-inc.com/software/software_page.html)).

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provided by M. E. Hervig was obtained from the GATS Scientific Software website ([http://gwest.gats-inc.com/software/software\\_page.html](http://gwest.gats-inc.com/software/software_page.html)). Work at the Jet Propulsion Laboratory, California Institute of Technology, was carried out under a contract with the National Aeronautics and Space Administration. This research was conducted as a component of the SPARC (Stratosphere-troposphere Processes And their Role in Climate) S-RIP activity, under the guidance and sponsorship of the World Climate Research Programme.

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**Table 1.** Reanalysis temperature data. Details are valid for the 100–10 hPa region and 2008–2013.

<u>Dataset</u>	<u>Horizontal resolution</u>	<u>Time resolution</u>	<u>Vertical resolution</u>	
<u>GEOS-5.9.1*</u>	<u>0.625° by 0.5°</u>	<u>3 hr</u>	<u>1.1–1.4 km</u>	<u>Rienecker et al. (2011)</u> <u>Goddard Earth Observing System Model, Version 5</u> <u>Near real time assimilation system</u> <u>Global Modeling and Assimilation Office</u> <u>NASA GMAO</u>
<u>MERRA**</u>	<u>0.666° by 0.5°</u>	<u>6 hr</u>	<u>1.1–1.4 km</u>	<u>Rienecker et al. (2011)</u> <u>Modern-Era Retrospective analysis for Research and Applications</u> <u>NASA GMAO</u>
<u>MERRA2</u>	<u>0.626° by 0.5°</u>	<u>3 hr</u>	<u>1.1–1.4 km</u>	<u>Gelaro et al. (2017)</u> <u>Modern-Era Retrospective analysis for Research and Applications Version 2</u> <u>NASA GMAO</u>
<u>JRA55</u>	<u>0.582° by 0.56°</u>	<u>6 hr</u>	<u>1.1–1.5 km</u>	<u>Kobayashi et al. (2015)</u> <u>Japanese 55-year Reanalysis</u> <u>Japanese Meteorological Agency (JMA)</u>
<u>ERA-I</u>	<u>0.75° by 0.75°</u>	<u>6 hr</u>	<u>1.2–1.5 km</u>	<u>Dee et al. (2011)</u> <u>European Centre for Medium-range Weather Forecasts (ECMWF) interim reanalysis</u> <u>ECMWF</u>
<u>NCEP-CFSR</u>	<u>0.5° by 0.5°</u>	<u>6 hr</u>	<u>2.3–4.8 km</u>	<u>Saha et al. (2010)</u> <u>National Centers for Environmental Prediction (NCEP)</u> <u>Climate Forecast System Reanalysis (CFSR)</u> <u>National Oceanic and Atmospheric Administration (NOAA)</u>

\*GEOS-5.9.1 is a near real-time assimilation product provided to the  
NASA Earth Observing System (EOS) instrument science teams.

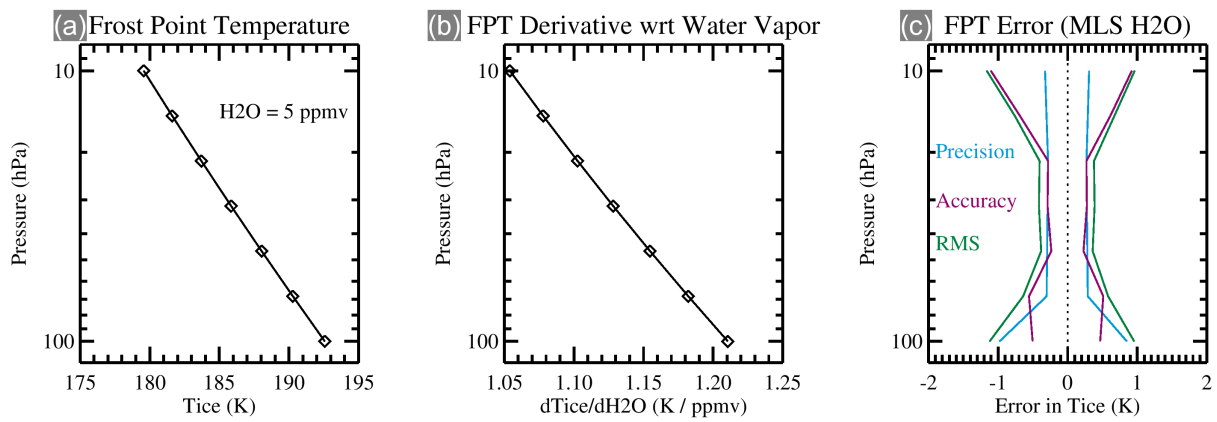
\*\* All except MERRA include GPS RO data during the time period studied here.

**Table 2.** Statistics of the reanalysis temperature distributions for LIQ PSCs relative to the theoretical STS equilibrium temperature ( $T_{eq}$ ) at 46 hPa for the combined 2008-2013 Antarctic winters (3261 profiles).

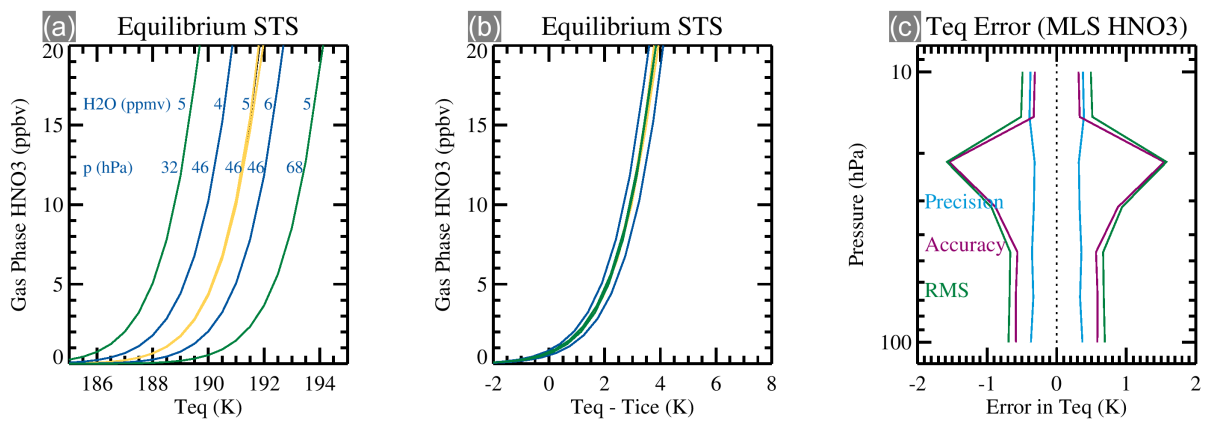
<u>Dataset</u>	<u>Median (K)</u>	<u>Mean (K)</u>	Standard Deviation (K)	Standard Error (K)	$\chi^2$
<u>GEOS5.9.1</u>	<u>-0.56</u>	<u>-0.57</u>	<u>0.54</u>	<u>0.009</u>	<u>1.62</u>
<u>MERRA</u>	<u>-0.90</u>	<u>-0.91</u>	<u>0.58</u>	<u>0.010</u>	<u>1.40</u>
<u>MERRA2</u>	<u>-0.54</u>	<u>-0.56</u>	<u>0.54</u>	<u>0.009</u>	<u>1.62</u>
<u>JRA55</u>	<u>-0.59</u>	<u>-0.62</u>	<u>0.53</u>	<u>0.009</u>	<u>2.21</u>
<u>ERA-I</u>	<u>-0.29</u>	<u>-0.32</u>	<u>0.57</u>	<u>0.010</u>	<u>2.08</u>
<u>NCEP-CFSR</u>	<u>-0.37</u>	<u>-0.38</u>	<u>0.59</u>	<u>0.010</u>	<u>1.82</u>

**Table 3.** As for Table 2, except for ICE PSCs relative to the theoretical ice frost point temperature (3288 profiles).

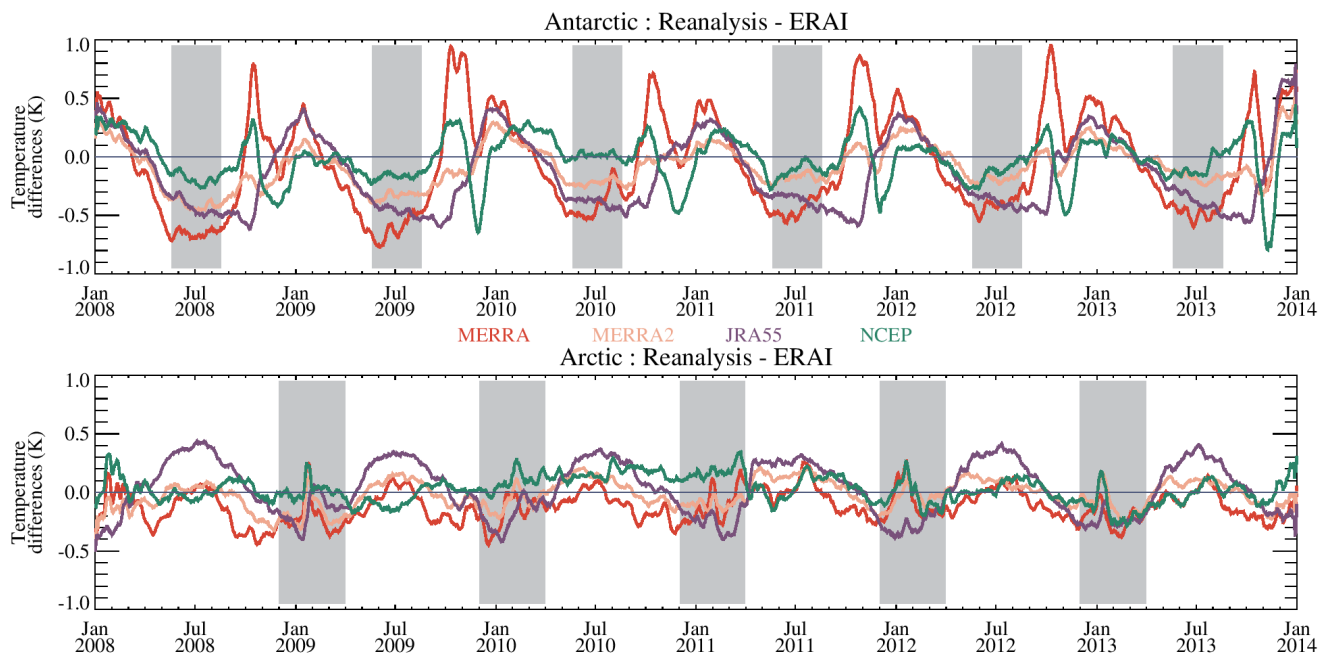
<u>Dataset</u>	<u>Median (K)</u>	<u>Mean (K)</u>	Standard Deviation (K)	Standard Error (K)	$\chi^2$
<u>GEOS5.9.1</u>	<u>-0.21</u>	<u>-0.18</u>	<u>0.71</u>	<u>0.012</u>	<u>1.94</u>
<u>MERRA</u>	<u>-0.58</u>	<u>-0.55</u>	<u>0.70</u>	<u>0.012</u>	<u>1.95</u>
<u>MERRA2</u>	<u>-0.23</u>	<u>-0.21</u>	<u>0.70</u>	<u>0.012</u>	<u>1.74</u>
<u>JRA55</u>	<u>-0.41</u>	<u>-0.38</u>	<u>0.70</u>	<u>0.012</u>	<u>1.56</u>
<u>ERA-I</u>	<u>+0.01</u>	<u>+0.03</u>	<u>0.72</u>	<u>0.013</u>	<u>1.54</u>
<u>NCEP-CFSR</u>	<u>-0.12</u>	<u>-0.11</u>	<u>0.73</u>	<u>0.013</u>	<u>1.64</u>



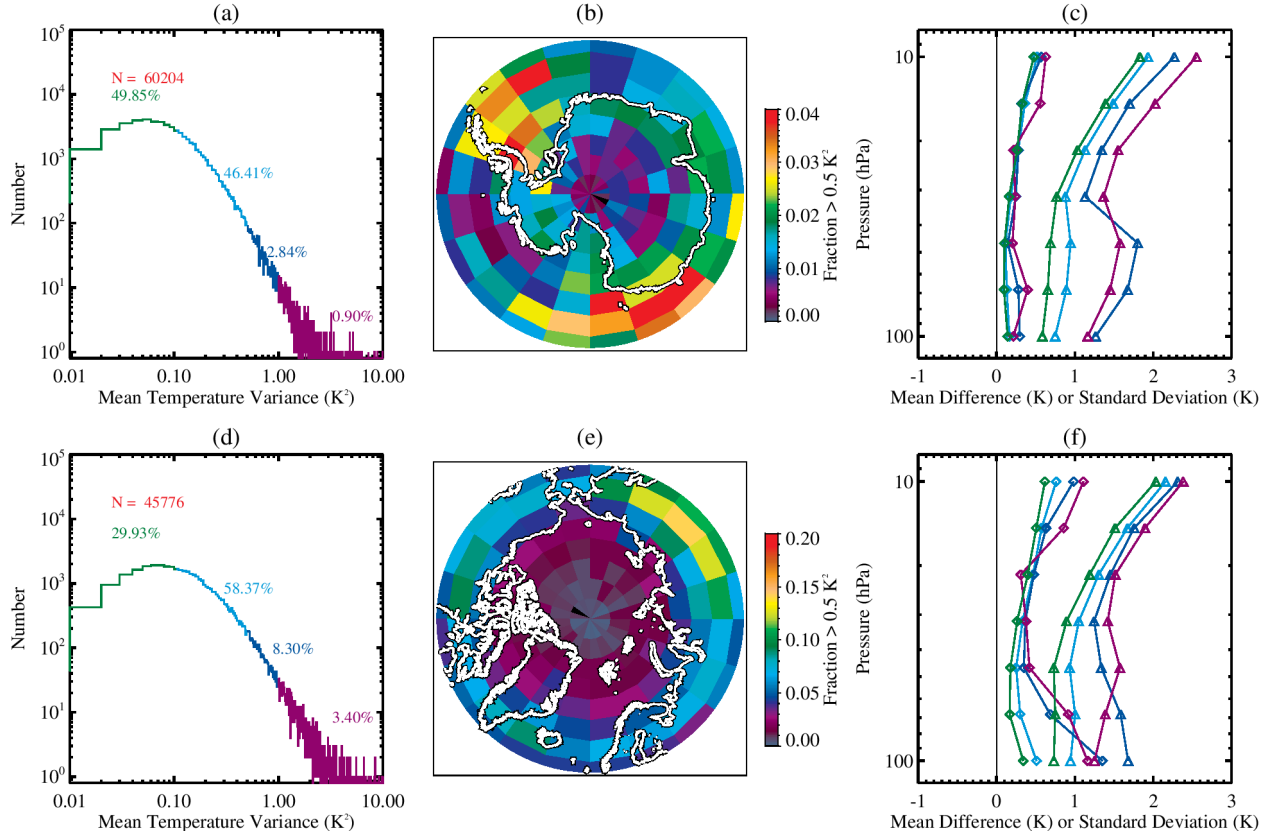
**Figure 1.** (a) Variation of frost point temperature with pressure in the lower stratosphere for a fixed  $H_2O$  volume mixing ratio (5 ppmv). (b) Derivative of the frost point temperature with respect to water vapor. (c) Error in determination of frost point temperature ( $T_{ice}$ ) arising from the uncertainties in the MLS  $H_2O$  measurement.



**Figure 2.** (a) Equilibrium HNO<sub>3</sub> uptake curves vs temperature for a variety of H<sub>2</sub>O mixing ratios (4, 5, 6 ppmv), H<sub>2</sub>SO<sub>4</sub> mixing ratios (0.1, 0.5 ppbv), and pressures (68, 46, 32 hPa). (b) As for (a), except for a coordinate transformation of the temperature scale relative to the ice frost point ( $T_{ice}$ ). (c) Error in the equilibrium STS temperature arising from the errors in the MLS HNO<sub>3</sub>.

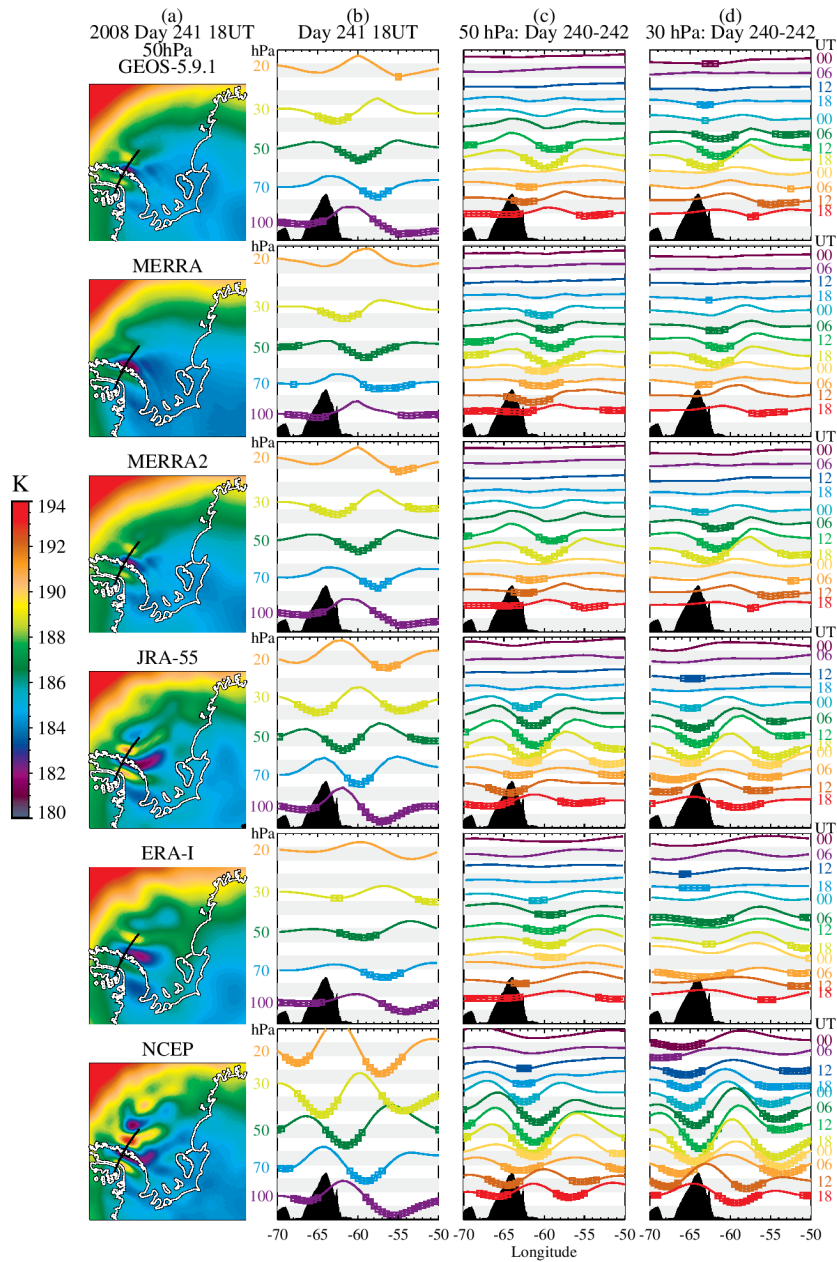


**Figure 3.** (Upper) Timeseries (for 12UT) from 2008 to 2013 of 10-day boxcar smoothed temperature differences for MERRA, MERRA2, JRA55 and NCEP-CFSR, relative to ERA-I at 46 hPa and averaged over the 60° Antarctic polar cap. The gray regions indicate the analysis periods defined for the analysis of PSC related metrics. (Lower) Similar, except for the Arctic.

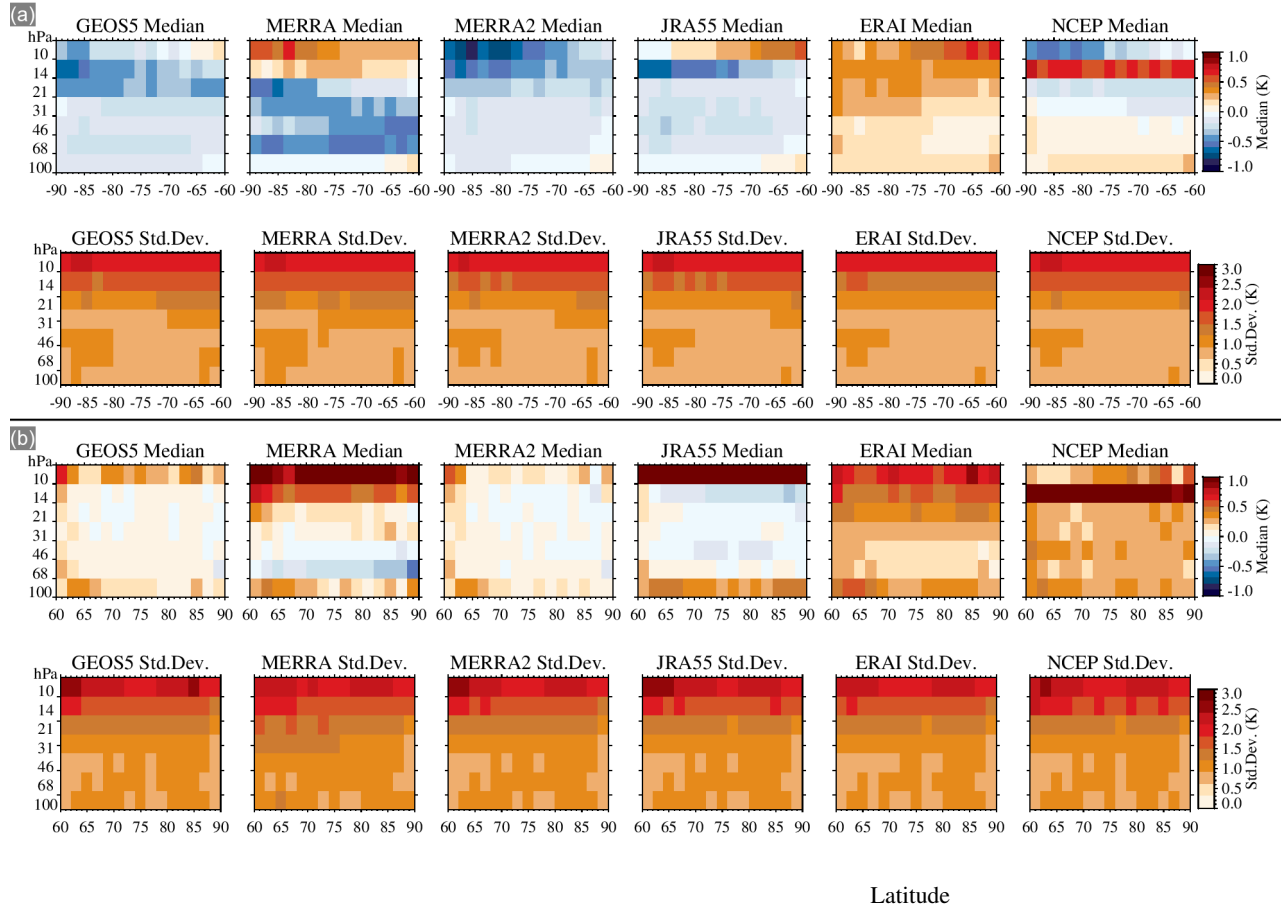


**Figure 4.** Temperature variance,  $\sigma^2 = \overline{T'^2}$ , in  $\text{K}^2$ , of the COSMIC profiles averaged over the pressure range 80–20 hPa for 2008–2013 for the Antarctic and Arctic. (a,d) Histogram of the mean COSMIC temperature variance with color coding for  $\sigma^2 \leq 0.1 \text{ K}^2$  (green),  $0.1 \text{ K}^2 > \sigma^2 \leq 0.5 \text{ K}^2$  (cyan),  $0.5 \text{ K}^2 > \sigma^2 \leq 1.0 \text{ K}^2$  (blue) and  $\sigma^2 \geq 1.0 \text{ K}^2$  (purple). N is the total number of profiles, and the percentages falling in each of the four colored  $\sigma^2$  regions are also given. (b,e) Geographic distribution of the fraction of COSMIC profiles with  $\sigma^2 > 0.5 \text{ K}^2$ . (c,f) Mean values (diamonds) and standard deviations (triangles) of the temperature differences between ERA-I and COSMIC, color coded for the COSMIC temperature variance as given in (a,d). The estimated noise variance is about  $0.03 \text{ K}^2$ .

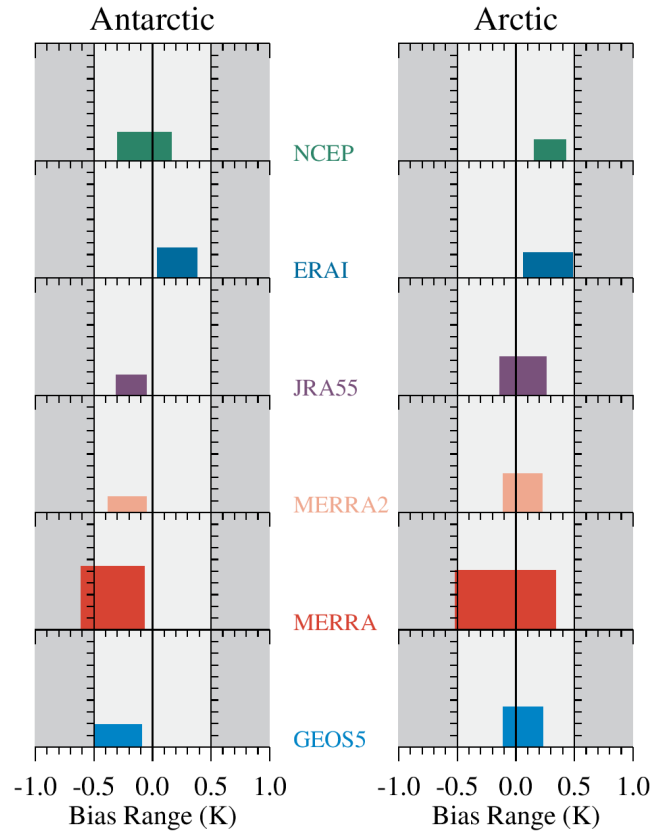




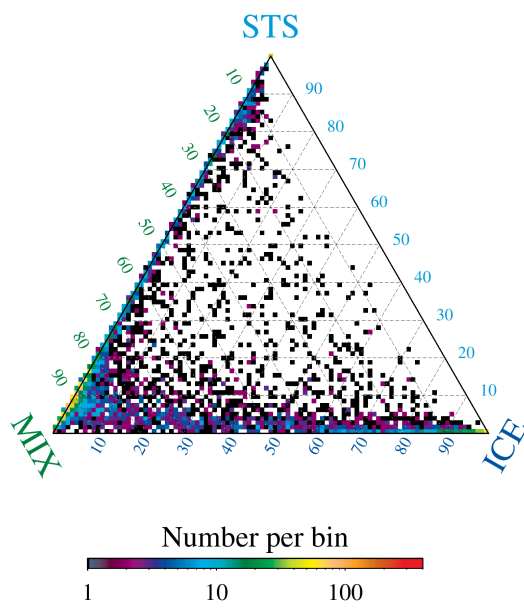
**Figure 5.** (a) Geographic distribution of 50 hPa temperatures over a region of the Palmer Peninsula on 28 August 2008 (day 241) at 18UT for different reanalyses. (b) Longitudinal reanalysis temperature structure from  $-70^{\circ}$  to  $-50^{\circ}$  on the 100, 70, 50, 30, and 20 hPa pressure levels along the  $72^{\circ}$  S latitude circle (shown as a black line in (a)). The ordinate is an arbitrary temperature scale with offset colored lines representing the longitudinal temperature variation for each of the labeled pressure levels. (c,d) Time series of the 50 hPa (30 hPa) reanalysis temperatures starting from 27 August (d240) at 0UT and ending on 29 August (d242) at 18UT. The ordinate is an arbitrary temperature scale with offset colored lines representing the temperature variation at the 6-hourly intervals labeled on the right. In (b,c,d), temperatures below the ice frost point are highlighted by square symbols, and mountain terrain is indicated by the black shading. Gray/white shading denotes both 5 K temperature bands and 500 m terrain increments.



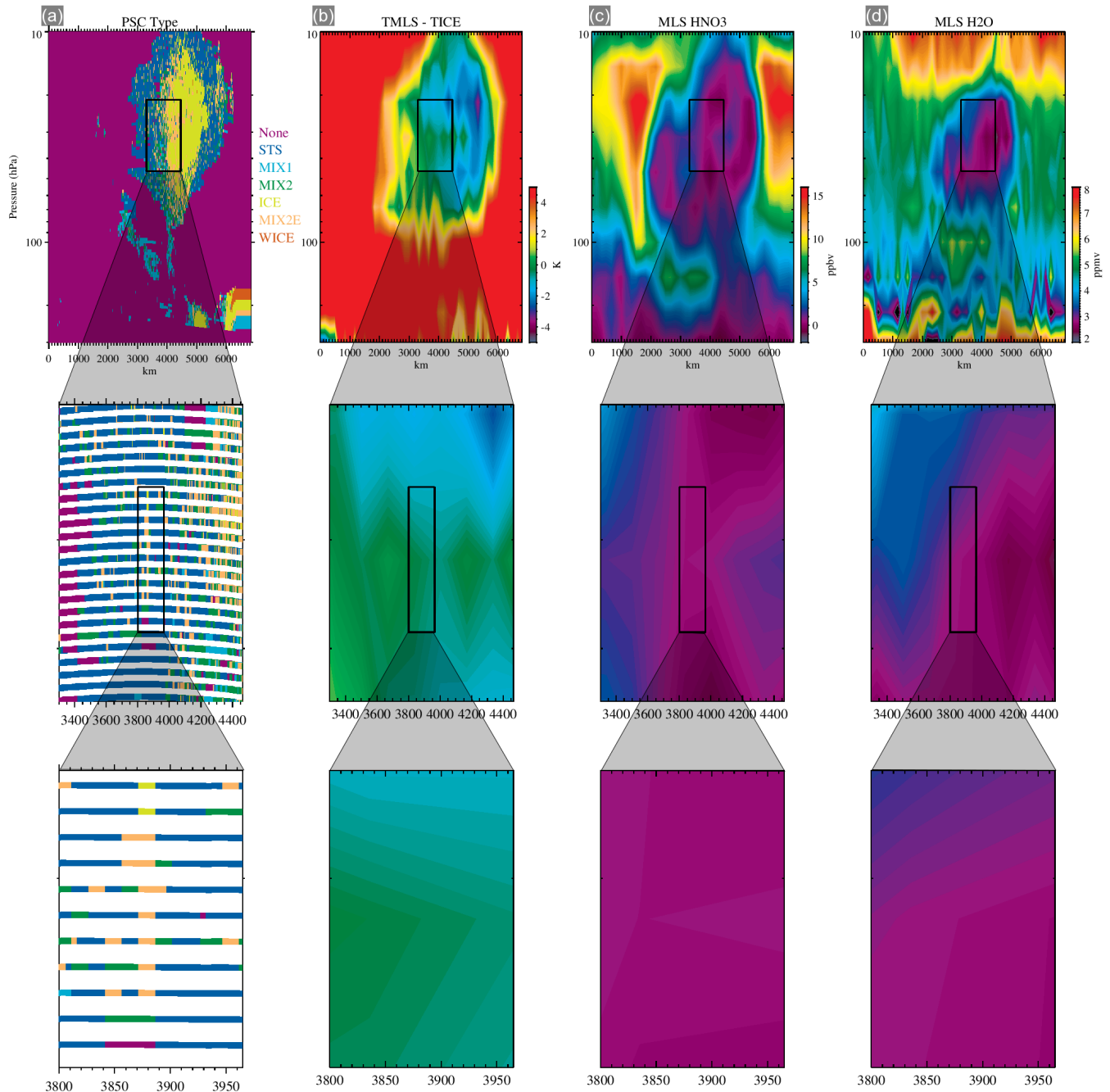
**Figure 6.** Zonal distributions of the median and standard deviations of the differences between the reanalysis temperatures and COSMIC temperatures ( $T_{re} - T_{COSMIC\ RO}$ ) averaged over 2008–2013 for (a) the Antarctic (90° S–60° S) and (b) the Arctic (60° N–90° N).



**Figure 7.** Temperature bias ranges of the reanalyses relative to COSMIC GPS RO for Antarctic and Arctic winters 2008–2013, poleward of 60°, and for pressure levels 68–21 hPa, derived from the data in Figure 6. The bias ranges are obtained from the extrema of the individual yearly mean bias values over 68–21 hPa. Each colored box indicates the bias ranges for the particular reanalysis scheme given in the legend; the abscissa gives the range of minimum to maximum bias; the ordinate gives the largest meridional bias range. Light grey shading indicates a  $\pm 0.5$  K scale in the bias range and a 0–1 K scale for the meridional bias range.

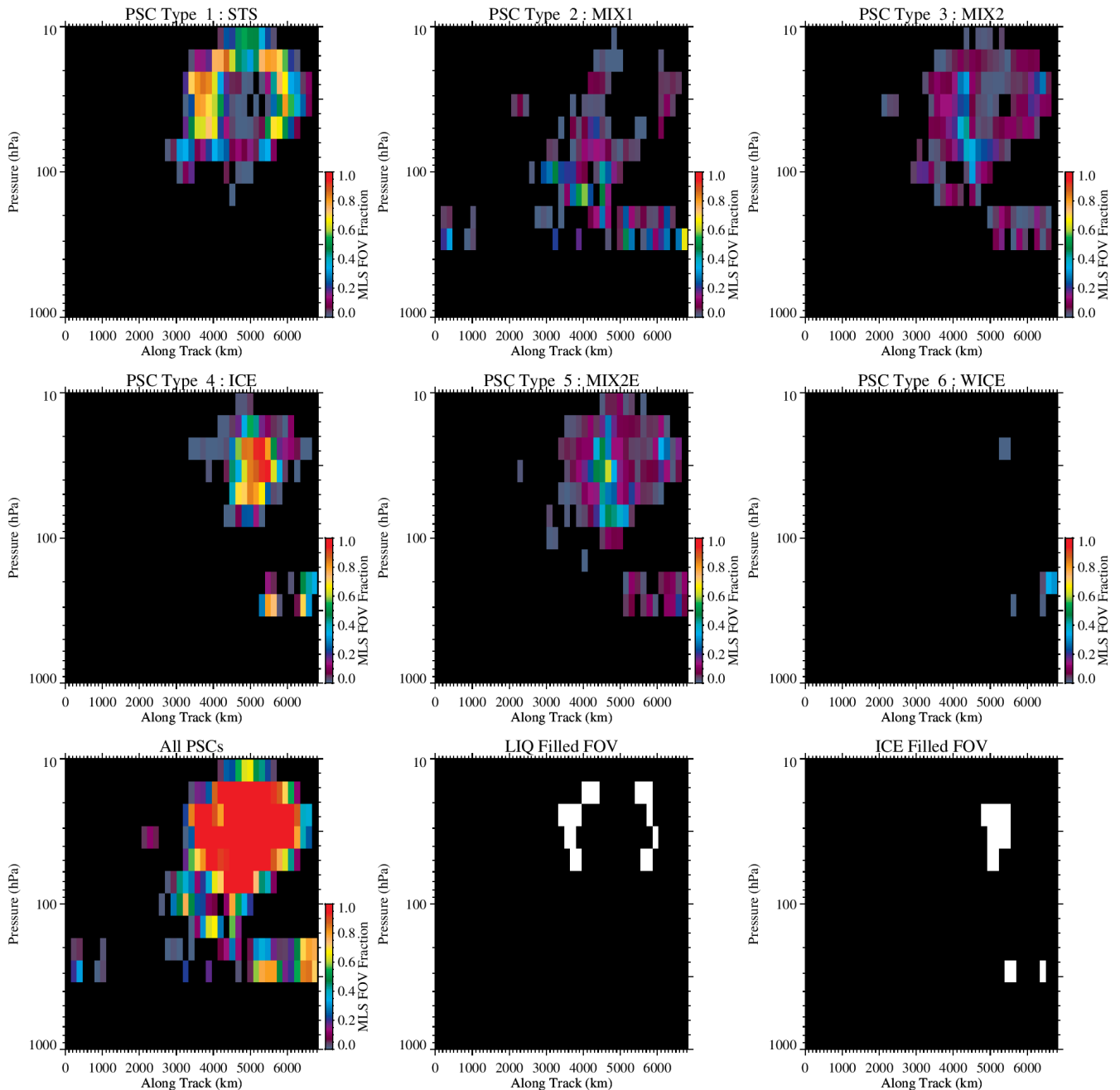


**Figure 8.** Ternary density plot of the relative proportions of STS/MIX/ICE occurring in the MLS geometric FOV at temperatures below the ice frost point for the 2013 Antarctic winter at 46 hPa.

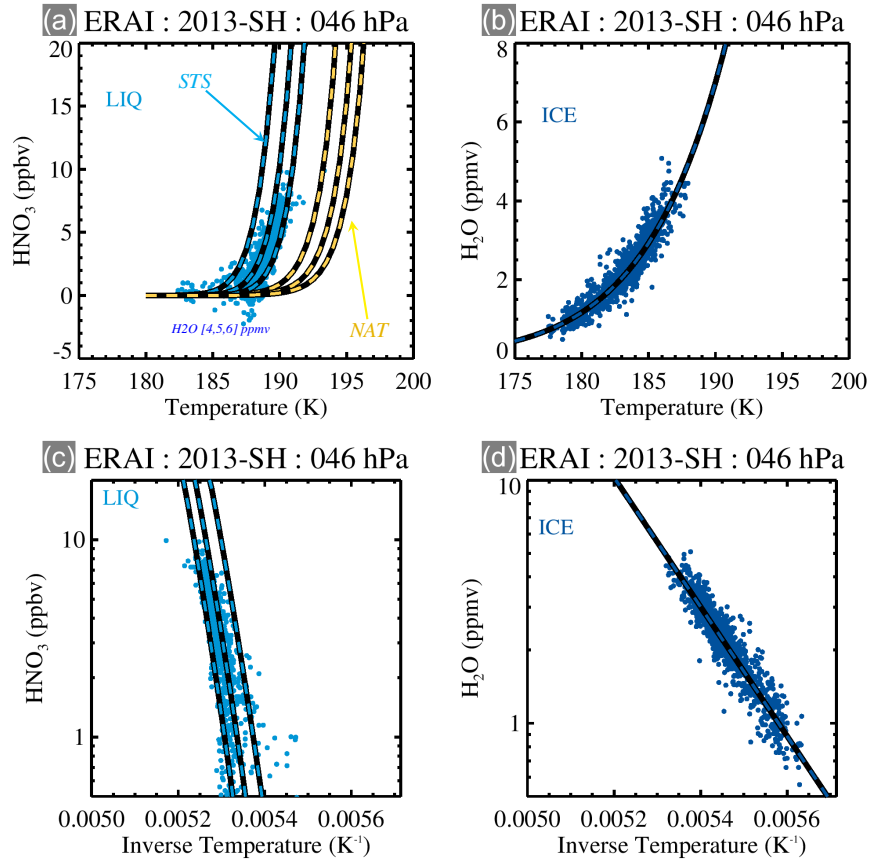


**Figure 9.** Along-track vertical cross-sections of PSCs, temperature,  $\text{HNO}_3$  and  $\text{H}_2\text{O}$  over a 7000 km transect crossing Antarctica on 23 June 2008 (2008d175). Column (a) CALIOP PSC types. Column (b) MLS temperature relative to the ice frost point. Column (c) MLS  $\text{HNO}_3$ . Column (d) MLS  $\text{H}_2\text{O}$ . Selected regions (black rectangular boxes), centered at 32 hPa in the top row, are shown enlarged in the middle row (1165 km along-track by 4.32 km high), and similarly enlarged again in the bottom row (165 km by 2.16 km). In the bottom row, the resolution is that of the MLS geometric FOV, in which MLS reports only a single measurement value, whereas CALIOP reports  $\sim 400$  individual 5 km by 0.180 km pixels.

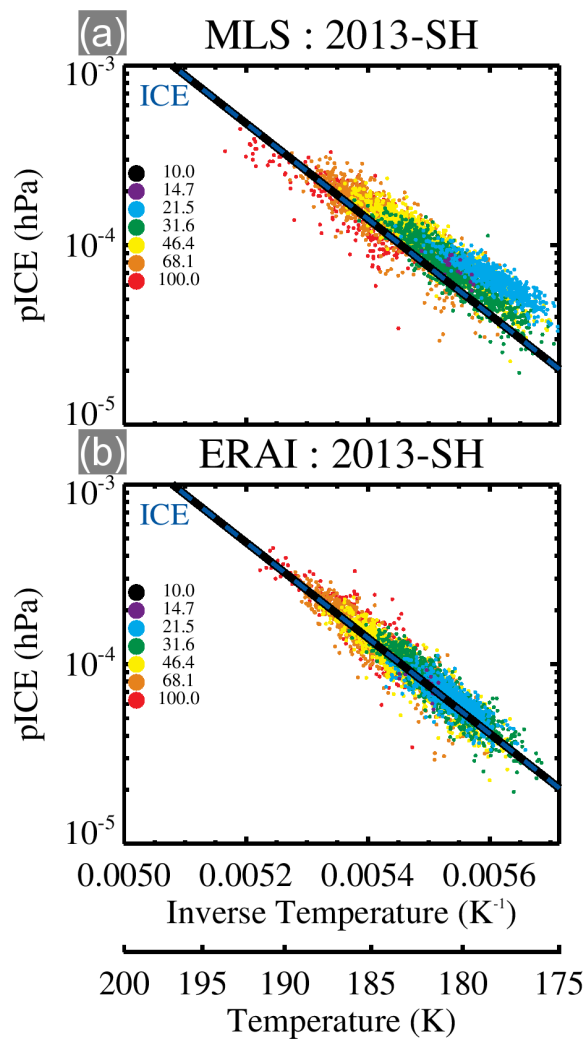
Antarctic CALIOP-orbit transect corresponding to the 165 km by 2.16 km-MLS geometric FOV-scenes (bottom row) centered at 32 hPa in Figure 9. (a) CALIOP-PSC Type. All types except wave ice are present in this scene consisting of STS:68.9%, ICE:1.6%, MIX1:0.6%, MIX2:12.9%, and MIX2E:13.2%. Clear sky cases (None, purple squares) make up the remaining 2.8%. (b) PSC Feature Mask N1 encodes the PSC-presence and height for each pixel relative to the local tropopause. All PSC-detections (orange-squares) are at least 4 km above the tropopause. The few pixels containing no PSC-detections (purple squares) are also 4 km or more above the local tropopause. (c) PSC Feature Mask N2N3 encodes the horizontal averaging and backscatter threshold (total backscatter ( $R_T$ )) or perpendicular ( $\beta_{perp}$ ) used for detection with the color-codings given in the legend.



**Figure 10.** Orbit transect from Figure 9 indicating the fraction of the MLS geometric FOV that is filled by each CALIOP classified PSC type and all PSCs. The white areas in the LIQ and ICE Filled FOV plots indicate the locations that pass the strict FOV filling criteria given in the

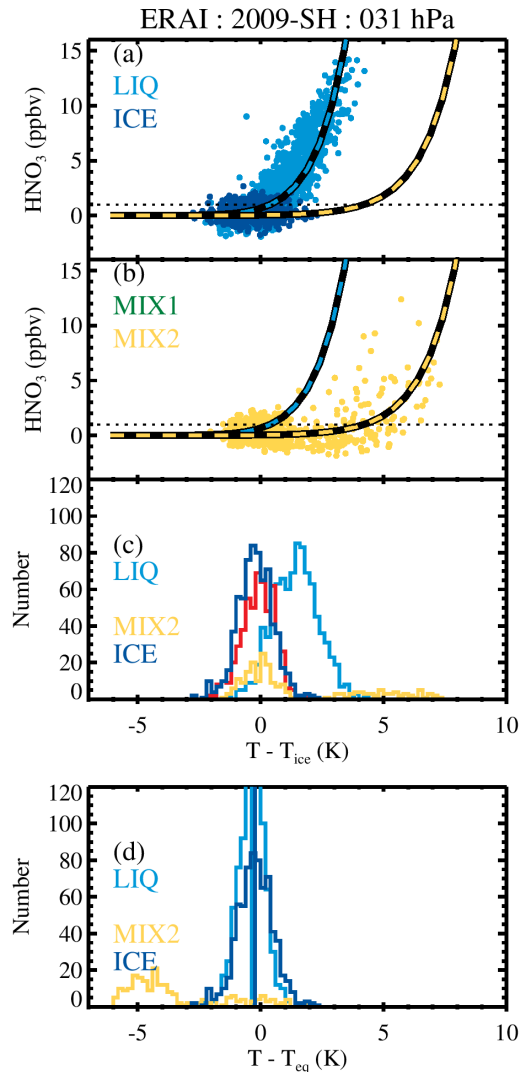


**Figure 11.** Scatter plots of coincident MLS HNO<sub>3</sub> and H<sub>2</sub>O vs ERA-I temperature for PSCs classified by CALIOP on the 46 hPa pressure level in the 2013 Antarctic winter. (a) MLS HNO<sub>3</sub> vs ERA-I temperature for liquid (LIQ) PSCs. The theoretical equilibrium uptake of HNO<sub>3</sub> by STS is shown for representative ambient H<sub>2</sub>O values by the cyan-black dashed lines. The yellow-black dashed lines show the corresponding NAT equilibrium curves. (b) MLS H<sub>2</sub>O vs ERA-I temperature for ice (ICE) PSCs. The blue-black dashed lines indicate the theoretical equilibrium for the frost point temperatures. (c,d) As for (a,b), except plotted as log mixing ratio vs inverse temperature.



**Figure 12.** Temperature variation of the estimated partial pressure of water vapor over ice,  $p_{ice}$ , determined from the product of the MLS  $H_2O$  volume mixing ratio and the total atmospheric pressure, for Antarctic ice PSCs in 2013. The pressure levels (hPa) are color coded and given in the legend. (a) MLS temperature. (b) ERA-I temperature. The blue-black dashed lines indicate the theoretical equilibrium  $p_{ice}$  as a function of the frost point temperature.

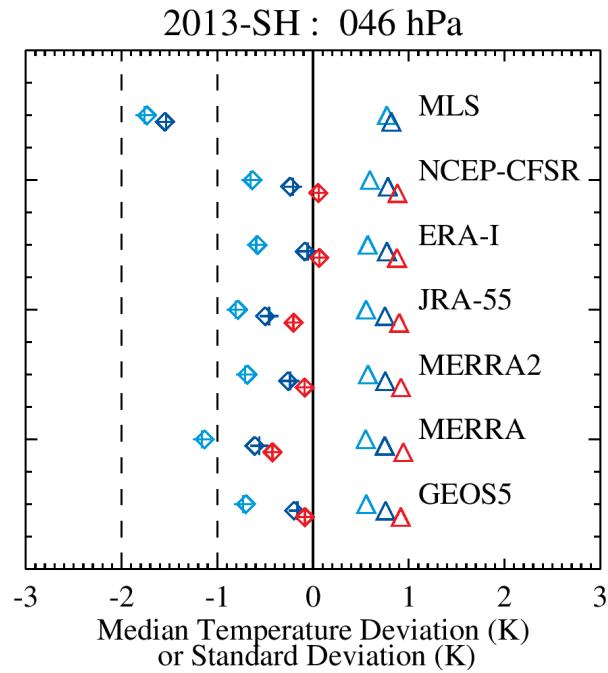




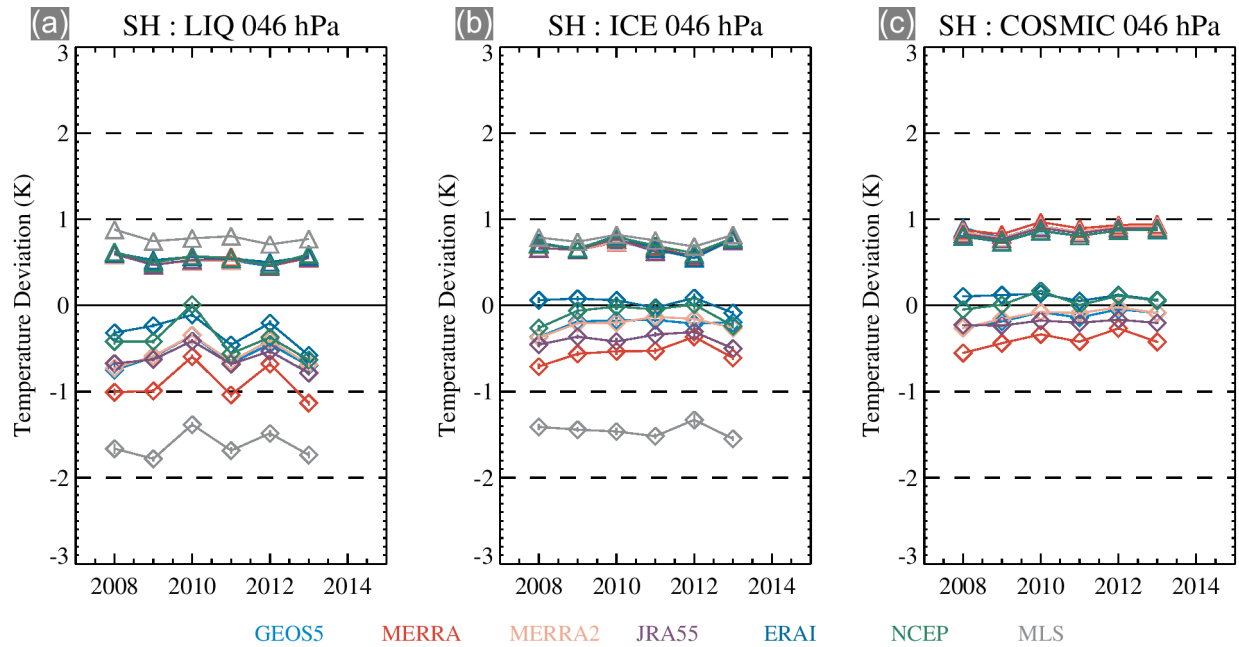
**Figure 13.** Composite statistics for d140–d230 (the bulk of the PSC formation period) of a representative year (2009) of the MLS gas-phase  $\text{HNO}_3$  variation with ERA-I temperature corresponding to CALIOP PSC classifications at 32 hPa, with the added constraint that at least 75% of the MLS FOV is filled with the same classification. (a) Scatter plot of  $\text{HNO}_3$  vs temperature deviation from the frost point ( $T - T_{\text{ice}}$ ) for PSCs classified as LIQ (cyan) and ICE (blue). (b) As for (a), but for MIX2 PSCs (yellow; because of non-equilibrium effects, which cause larger temperature scatter, MIX2 PSCs are not used in this analysis, but this panel is shown to indicate the good discrimination between the solid and liquid uptake curve branches.) Equilibrium STS (black/cyan dashed) and NAT (black/yellow dashed) curves show the theoretical uptake of  $\text{HNO}_3$ . (c) Temperature histograms for  $\text{HNO}_3$  mixing ratio  $>1$  ppbv for LIQ PSC type; data in the ICE classification are not subject to this constraint. The red histogram indicates the distribution of LIQ PSCs that have  $\text{HNO}_3$  below the 1 ppbv threshold. (d) Temperatures transformed according to the STS equilibrium curve for the LIQ classification and NAT equilibrium curve for the MIX2 classification; the ICE classification remains the same as in (c) for comparison.

Histograms and statistics of the reanalysis temperature distributions for LIQ PSCs relative to the theoretical STS equilibrium temperature ( $T_{eq}$ ) at 46 hPa for the combined 2008-2013 Antarctic winters. A normal distribution curve is superposed on each reanalysis histogram, with the corresponding mean and standard deviation given in the legend:

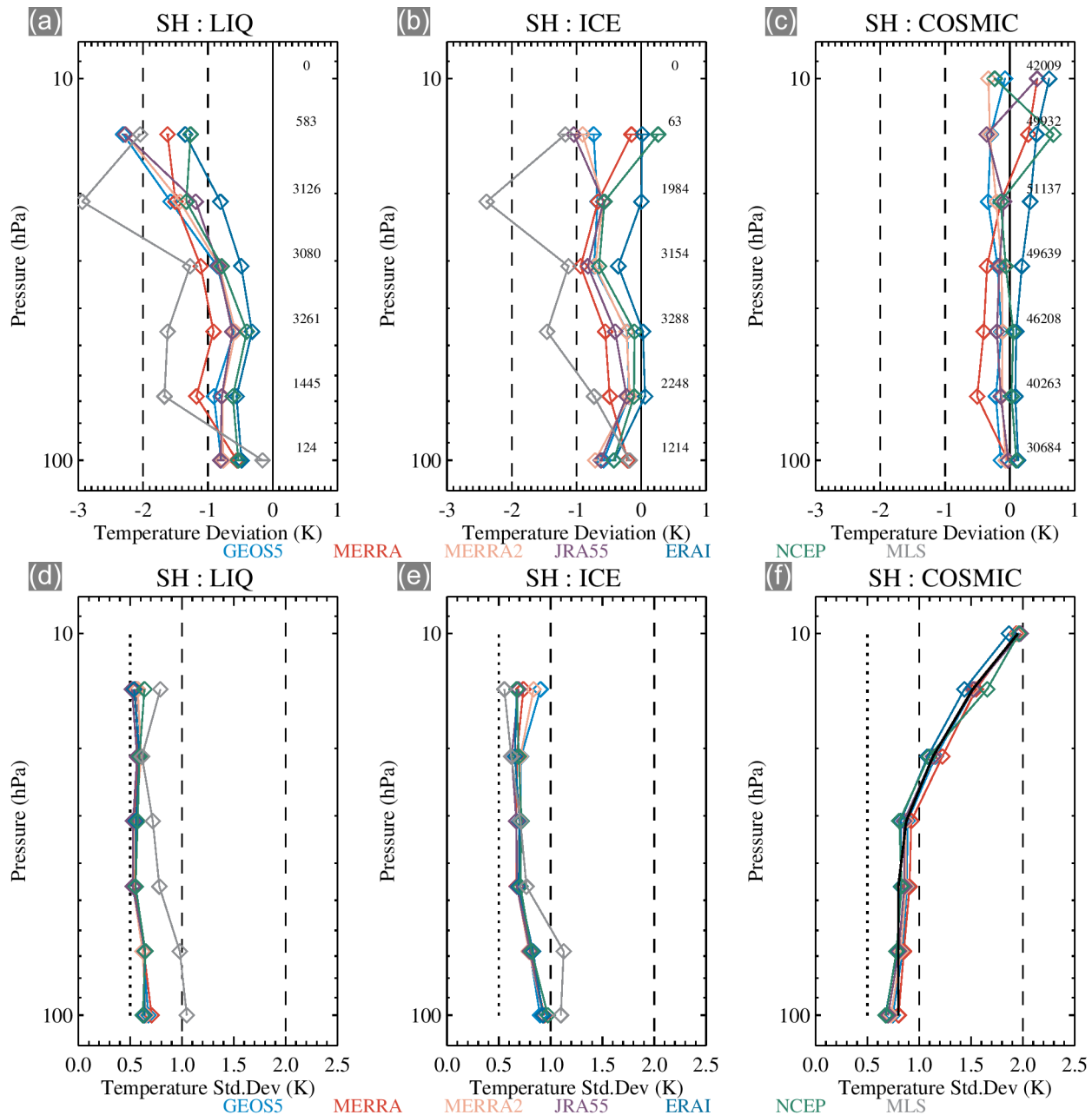
As for Figure ??, except for ICE PSCs relative to the theoretical ice frost point temperature:



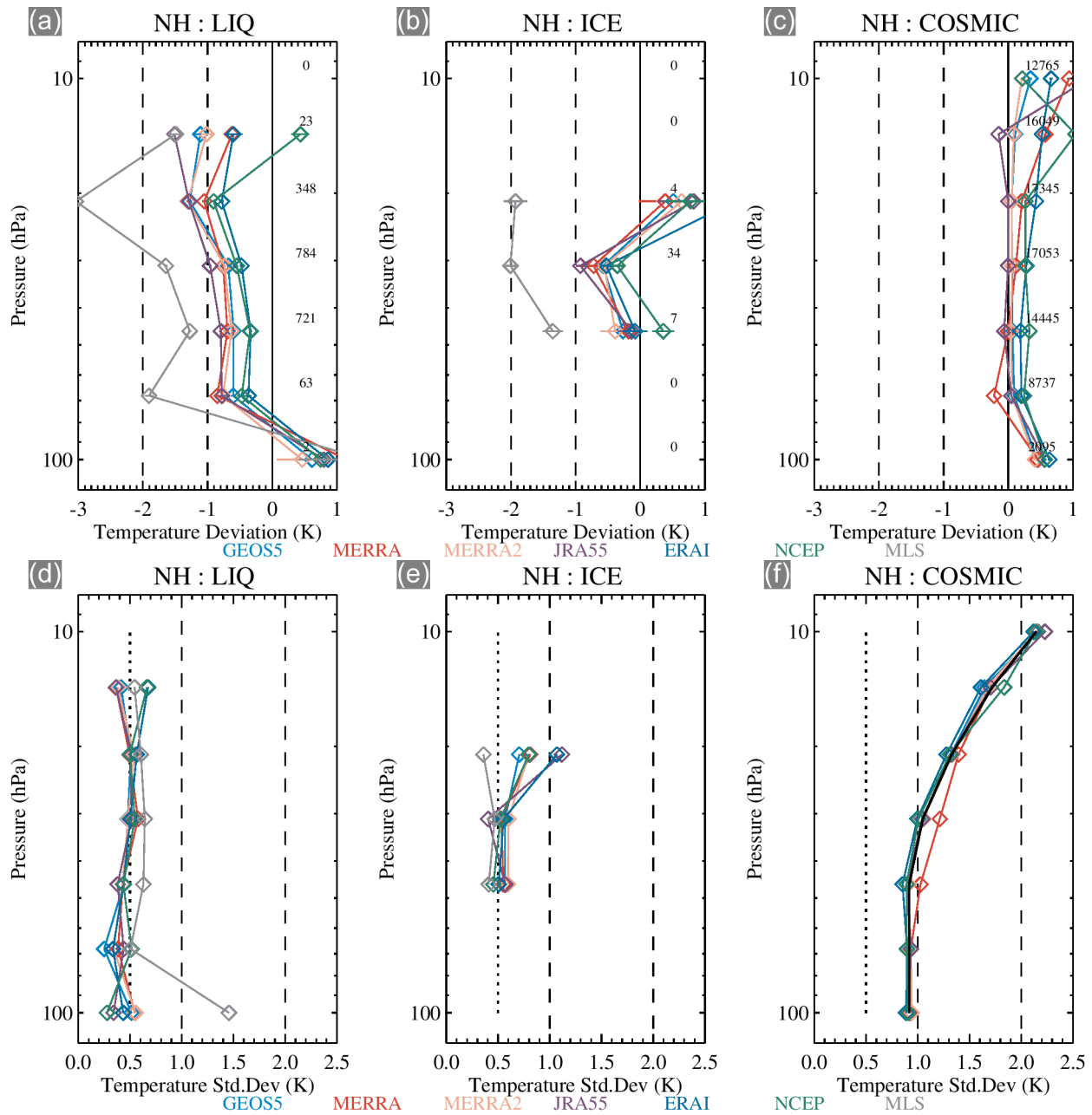
**Figure 14.** Median deviations (diamonds) and standard deviations (triangles) of the temperature distributions for LIQ (cyan), ICE (blue) and COSMIC (red) for each reanalysis, GEOS-5.9.1, and MLS, for a representative year (2013) at 46 hPa. The plus symbols denote the means of the distributions. Their similarity to the median values indicates that the distributions have small skewness.



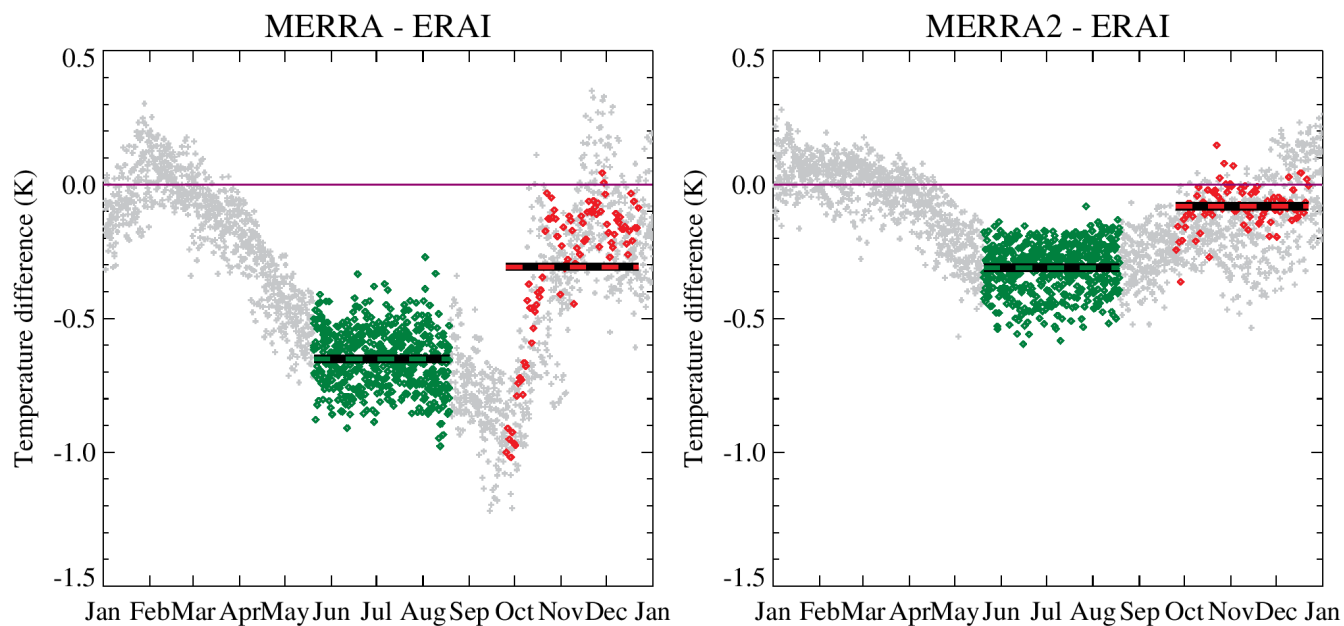
**Figure 15.** Median temperature deviations (diamonds) from  $T_{eq}$  for (a) LIQ PSCs and from  $T_{ice}$  for (b) ICE PSCs for the temperature distributions in each year 2008–2013 at 46 hPa. The standard deviations of the temperature deviations are also shown (triangles). Lines for the different reanalyses, GEOS-5.9.1, and MLS are color coded (see legend). (c) as for (a,b) except for deviations with respect to COSMIC GPS RO.



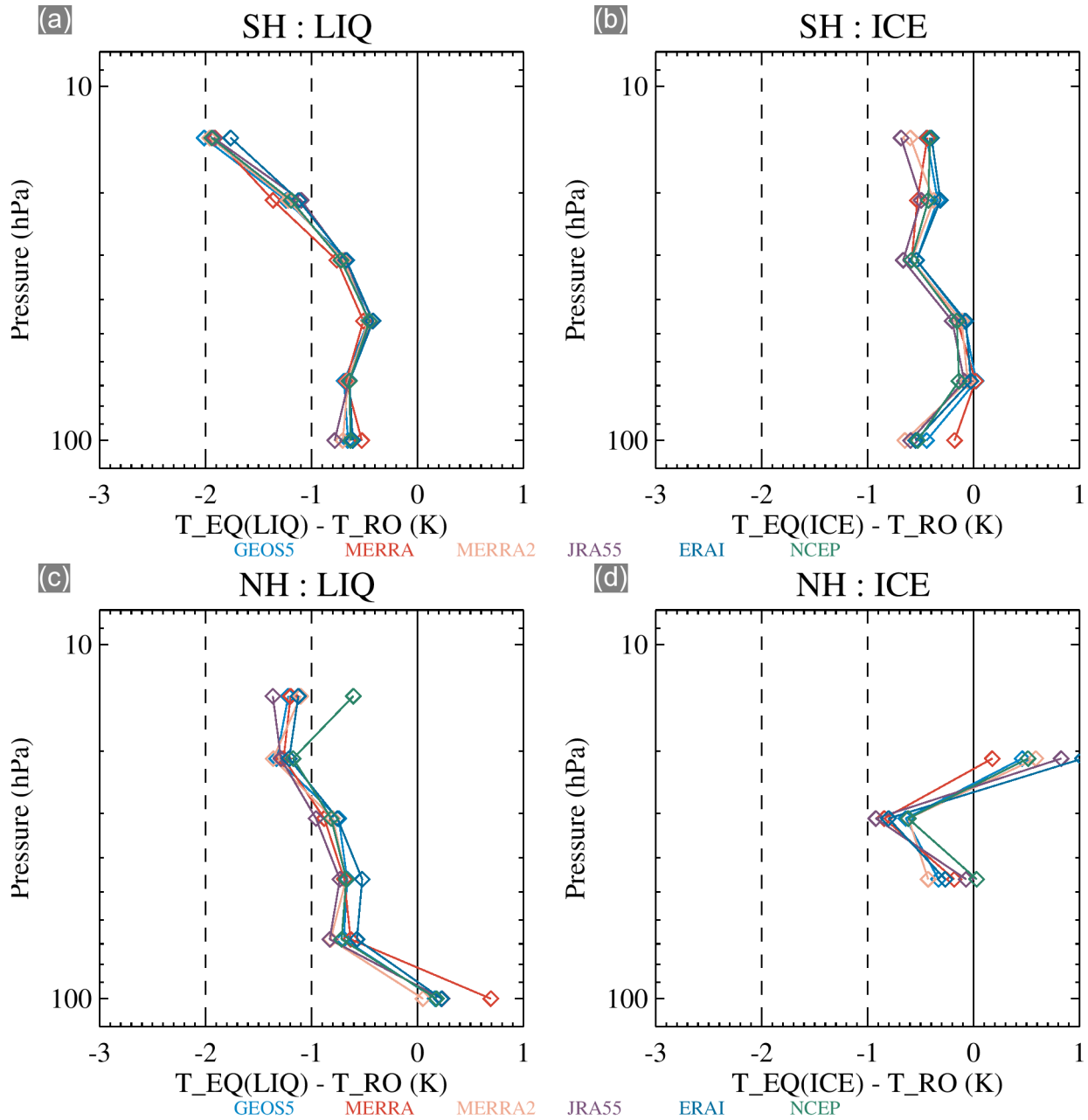
**Figure 16.** Vertical profiles of median temperature deviations from  $T_{eq}$  for (a) LIQ PSCs and for (b) ICE PSCs for the temperature distributions accumulated over the Antarctic PSC seasons (20 May (d140) to 18 August (d230) from 2008 to 2013). Lines for the different reanalyses, GEOS-5.9.1, and MLS are color coded (see legend); the numerical values on the right-hand side of each panel indicate the total number of observations in the distribution at the corresponding pressure level. (c) as for (a,b) except for deviations with respect to COSMIC GPS RO. (d,e,f) The standard deviations of the corresponding temperature distributions shown in (a,b,c). Dotted lines indicate a standard deviation of 0.5 K



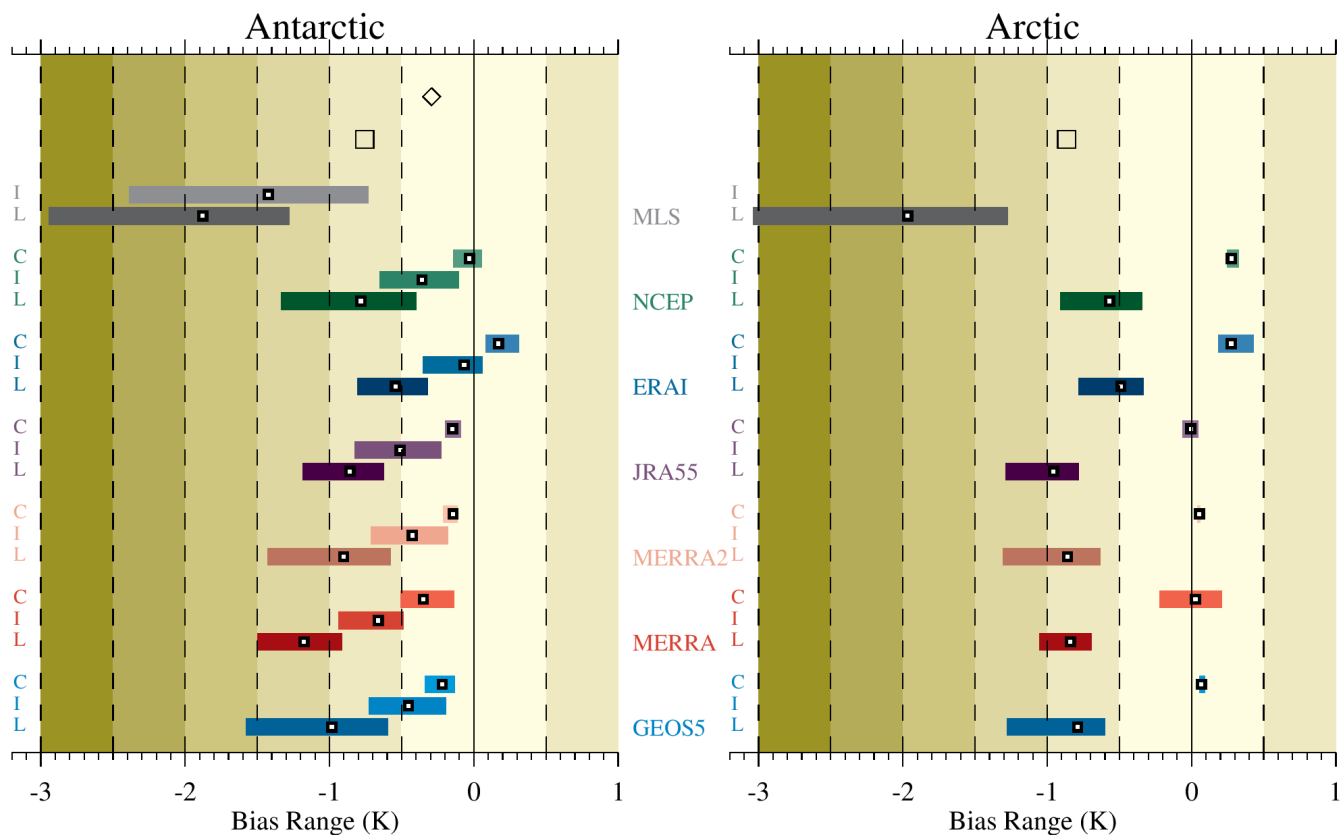
**Figure 17.** As for Figure 16, except for the Arctic PSC seasons (2 December (d336) to 31 March (d090) from 2008/2009 to 2012/2013).



**Figure 18.** Daily mean temperature differences (not smoothed) of MERRA (left) and MERRA-2 (right) relative to ERA-I at 62 hPa (representative of the balloon float heights) in the 60° Antarctic polar cap for 2008–2013. Green-black dashed line indicates the mean of the 2008–2013 differences (green symbols) in the PSC analysis window. Red-black dashed line indicates the mean of the differences (red symbols) over the time-span of 90% of the balloon measurements.



**Figure 19.** Vertical profiles of the temperature differences between (a) LIQ equilibrium and COSMIC GPS RO,  $\overline{\Delta T_{LIQ}} - \overline{\Delta T_{COSMIC}}$ , and (b) ICE equilibrium and COSMIC RO,  $\overline{\Delta T_{ICE}} - \overline{\Delta T_{COSMIC}}$ , for the Antarctic. (c,d) As for (a,b) except for the Arctic. Lines for the different reanalyses are color coded according to the legend.



**Figure 20.** Temperature bias ranges of the reanalyses, and MLS, relative to the LIQ (L) and ICE (I) equilibrium references, and COSMIC (C), for Antarctic and Arctic winters 2008–2013, poleward of 60°, and for pressure levels from 68–21 hPa, derived from the data in Figures 16 and 17. The bias ranges are obtained from the extrema of the weighted yearly mean bias values over 68–21 hPa weighted by the yearly standard deviations. Each horizontal colored bar indicates the range of the minimum to maximum bias for MLS and the particular reanalysis scheme given in the legend. White squares with black border indicate the mean bias over 68–21 hPa. Open square (diamond) symbols indicate the mean values of  $\Delta T_{\text{LIQ}} - \Delta T_{\text{COSMIC}}$  ( $\Delta T_{\text{ICE}} - \Delta T_{\text{COSMIC}}$ ) over 68–21 hPa, obtained from Figure 19. There are insufficient statistics for a reliable comparison with the ICE reference in the Arctic. Note that MLS has not been compared directly to COSMIC. Background shading indicates 0.5 K increments in the bias range.