Algorithm Stability and the Long-Term Geospace Data Record from TIMED/SABER

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Abstract

The ability of satellite instruments to accurately observe long-term changes in atmospheric temperature depends on many factors including the absolute accuracy of the measurement, the stability of the calibration of the instrument, the stability of the satellite orbit, and the stability of the numerical algorithm that produces the temperature data. We present an example of algorithm instability recently discovered in the temperature dataset from the SABER instrument on the NASA TIMED satellite. The instability resulted in derived temperatures that were substantially colder than anticipated from mid-December 2019 to mid-2022. This algorithm-induced change in temperature over one to two years corresponded to the expected change over several decades from increasing anthropogenic CO2. This paper highlights the importance of algorithm stability in developing Geospace Data Records (GDRs) for Earth's mesosphere and lower thermosphere. A corrected version (Version 2.08) of the temperatures from SABER is described.

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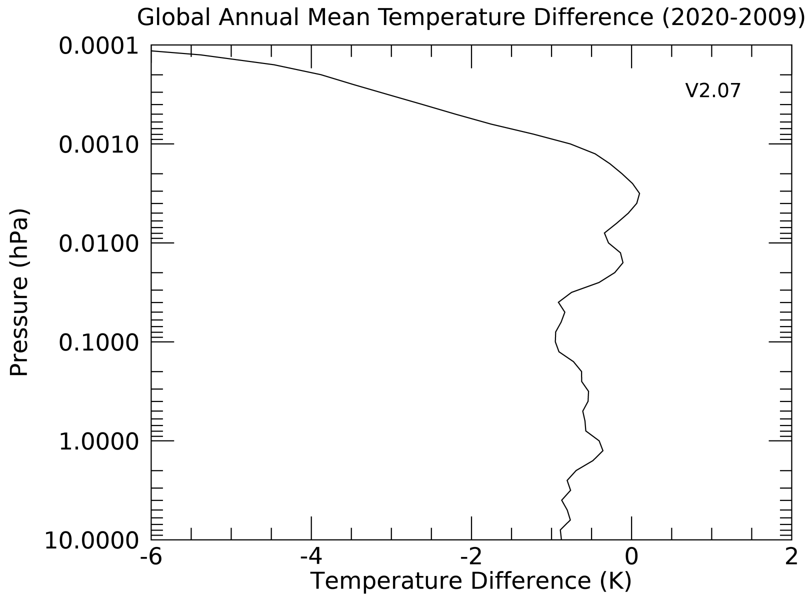
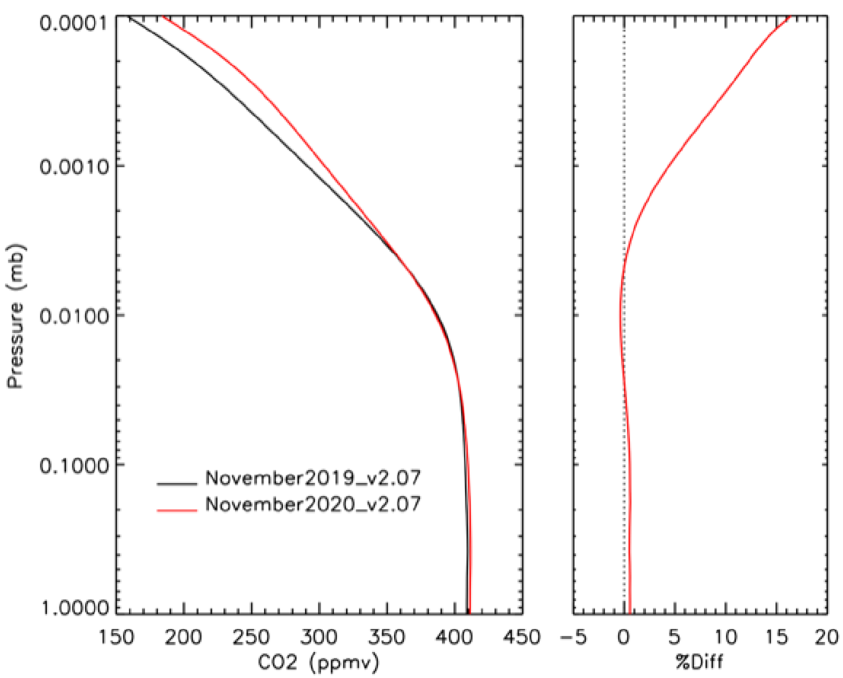
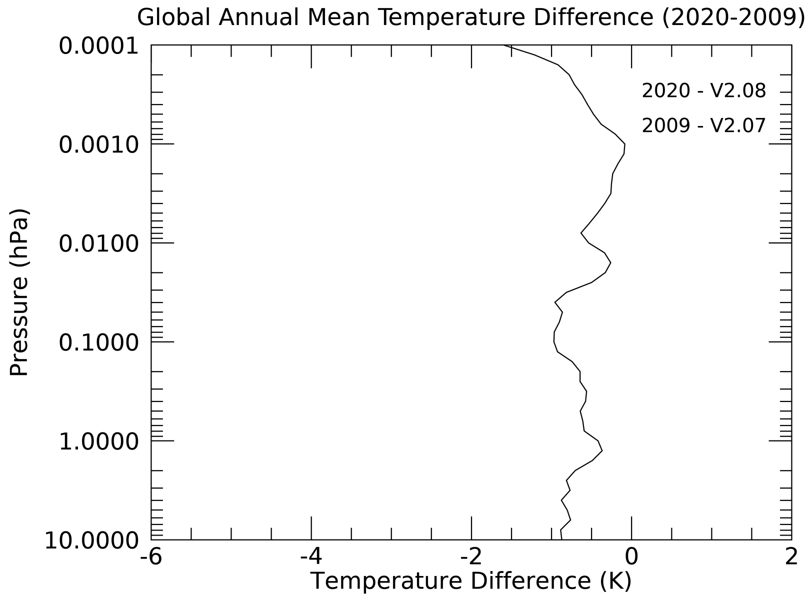

Global Annual Mean Temperature Difference (2020-2009)
V2.07
Pressure (hPa)
Temperature Difference (K)


Pressure (mb)
November2019_v2.07
November2020_v2.07
CO2 (ppmv)
%Diff



Global Annual Mean Temperature Difference (2020-2009)
2020 - V2.08
2009 - V2.07
Pressure (hPa)
0.0001
0.0010
0.0100
0.1000
1.0000
10.0000
-6
-4
-2
0
2
Temperature Difference (K)

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Abstract. The ability of satellite instruments to accurately observe long-term changes in atmospheric temperature depends on many factors including the absolute accuracy of the measurement, the stability of the calibration of the instrument, the stability of the satellite orbit, and the stability of the numerical algorithm that produces the temperature data. We present an example of algorithm instability recently discovered in the temperature dataset from the SABER instrument on the NASA TIMED satellite. The instability resulted in derived temperatures that were substantially colder than anticipated from mid-December 2019 to mid-2022. This algorithm-induced change in temperature over one to two years corresponded to the expected change over several decades from increasing anthropogenic CO_2. This paper highlights the importance of algorithm stability in developing *Geospace Data Records* (GDRs) for Earth's mesosphere and lower thermosphere. A corrected version (Version 2.08) of the temperatures from SABER is described.

Plain Language Summary. Instruments on Earth orbiting satellites offer the opportunity to detect long-term changes in atmospheric temperature. Many factors may affect the ability to identify actual long-term changes in the temperature and to distinguish these from changes in the instrument or from unintended changes in the algorithm that produces the temperature data from the instrument observations. SABER is an instrument on a NASA satellite that has been observing temperatures from 15 km to 110 km (10 to 70 miles) in altitude for over 20 years. An 'instability' in the scientific algorithm used to derive temperature from the instrument observations was recently discovered, beginning in late 2019. An unintended change was made in a parameter central to the derivation of temperature from SABER measurements. The consequence was that the atmospheric temperatures between 85 km and 110 km (51 to 68 miles) from 2020 onward were several degrees colder than they would have been without the unintended change. This has been corrected and an updated version of the SABER temperatures and all other SABER data products, called Version 2.08, is now publicly available.

Key Points

1. The concept of Geospace Data Records (GDRs) and their relevance to accurate detection of long-term change is introduced.

2. Algorithm instability in a GDR of the 20-year record of SABER temperatures between 85 km and 110 km is described and corrected.

3. The field of Geospace Climate is emerging as a frontier with scientific and economic relevance. Accurate GDRs are essential to both.

1. Introduction

We begin by defining the concept of a Geospace Data Record (GDR). The term GDR is derived from the commonly used Climate Data Record (CDR) of tropospheric climate science. The definition of a CDR is "a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change" (National Research Council, 2004). We adopt this definition almost verbatim for a GDR by substituting the word 'geospace' for 'climate.' Geospace is further defined as broadly the region between the mesosphere and the exosphere (roughly 60 km to above 600 km) where the atmosphere and space environment interact, and both are subject to the variability of solar ultraviolet and extreme ultraviolet radiation, as well as to particle precipitation. Geospace is undergoing long-term change due to increasing carbon dioxide (e.g., Mlynczak, Hunt, et al., 2022 and references therein) as predicted over 30 years ago (Roble and Dickinson, 1989; Cicerone, 1990). These changes are expected to be factors in future space policy and space law decisions (e.g., orbit debris regulations and mitigation) and in general in the overall space economy (Mlynczak, Yue, et al., 2021; Bruinsma, Fredrizzi, et al., 2021). With both scientific inquiry and future economic policy in play, attention must be given to developing GDRs that can be used "to determine geospace variability and change." The long-running SABER data record of temperature, composition, and energetics of the stratosphere, mesosphere, and thermosphere is an example of a GDR. Understanding ongoing change in geospace due to increasing carbon dioxide (CO_2) and variable solar activity is at the forefront of science inquiry. Generation of high-quality GDRs is essential to understanding geospace change and separating it from the effects of natural variability of the Sun.

Many details must be carefully considered to develop and characterize a dataset obtained from satellite observations as a GDR (Mlynczak, Yue et al., 2021). We broadly define instability in a GDR as any change in the instrument or in the data processing that introduces an increase in the systematic error (and hence, a decrease in accuracy) of the GDR. These changes may be slow and difficult to detect, such as a steady degradation of an instrument's on-board calibration source. Long-term changes in the orbit of the satellite hosting an instrument may also induce spurious changes to a CDR or GDR if the scientific algorithm that produces the data is explicitly dependent on orbital parameters. An example of this is reviewed in Section 4. Other instabilities may be prompt, such as discussed here for the SABER instrument on the NASA TIMED satellite. A GDR with an undetected instability will have time-varying and false trends in its data record that will compromise its utility for scientific research or for informing societal decisions.

In this paper we review a recently discovered algorithm instability in the SABER temperature dataset. The instability was caused by a change in a key input to the SABER temperature retrieval algorithm, namely, the time series of the CO_2 concentration. The radiance measured by SABER from CO_2 at 15 μm depends primarily on temperature and the CO_2 abundance. The algorithm by which the temperature is derived computes limb radiances based on estimates of temperature and CO_2 compared with the measured radiance. The approach is iterative and converges when the combination of temperature and CO_2 used in radiative transfer calculations matches the observed radiance. The relationship of temperature and CO_2 to the measured radiance is an inverse one in the sense that more (less) CO_2 results in lower (higher) retrieved temperatures. Errors in CO_2 therefore translate directly into errors in the derived temperature. The changes introduced into the SABER temperature algorithm (described below) were as large as 15% at 1 x 10^{-4} hPa. These CO_2 changes introduced changes of 2 K to 6 K in temperature which corresponded to several decades of anticipated temperature trend due to anthropogenically increasing CO_2. These results highlight the attention that must be given when generating a scientifically useful CDR or GDR for any parameter. The instability has been removed as described below and a new version of SABER temperatures (and all other SABER parameters), Version 2.08, is described and publicly available.

Section 2 describes the SABER measurement technique. Section 3 defines and describes an occurrence of "algorithm instability" in the operational SABER (Version 2.07) temperatures. Section 4 is a Discussion and Summary to conclude the paper.

2. SABER Measurement Approach and Data Description

The SABER instrument, launched on the NASA TIMED satellite in December 2001 has been measuring the temperature of the stratosphere, mesosphere, and lower thermosphere (15 km to 110 km) uninterrupted since January 2002. SABER is a limb-scanning radiometer that measures infrared emission from the CO_2 molecule in two different spectral intervals in the 15-micrometer (μm) spectral region. This standard 'two-color' technique was developed by Gille and House (1971) and was successfully applied to retrieve stratospheric and lower mesospheric temperatures (at pressures between approximately 100 hPa and 0.1 hPa, 15 km to 65 km) from limb radiances measured by the Limb Radiance Inversion Radiometer (LRIR) instrument that flew on the Nimbus 6 satellite (Gille, Bailey et al., 1980) and the Limb Infrared Monitor of the Stratosphere (LIMS) instrument that flew on the Nimbus 7 satellite (Gille, Russell et al., 1984). The premise behind the two-color technique is that, if the vertical profile of CO_2 mixing ratio is known, measurements of infrared emission from CO_2 in the two spectrally different channels allow the vertical profile of temperature to be retrieved as a function of pressure. For the stratosphere and lower mesosphere, the mixing ratio of CO_2 is essentially constant (i.e., it is well-mixed) throughout, at or just slightly less than the mixing ratio at the Earth's surface. Both LRIR and LIMS used constant CO_2 mixing ratio profiles in their temperature derivations.

The CO_2 mixing ratio decreases from its well-mixed value above 65 km (0.1 hPa), due to diffusive separation, eddy diffusion, and photolysis (Garcia, Lopez-Puertas et al., 2014) and shown by Rinsland, Gunson et al. (1992) with data from the Atmospheric Trace Molecular Spectroscopy (ATMOS) instrument that flew on the Spacelab 3 mission aboard the Space Shuttle in 1985. The SABER instrument (proposed in 1992) is focused on the previously unexplored mesosphere and lower thermosphere region from 60 to 110 km. SABER employs the same two-channel approach with spectral intervals nearly identical to those on the LIMS instrument. However, SABER did not initially anticipate having an *operational* measurement of the CO_2 concentration to provide to the temperature retrieval process. At the time of proposal, modeling the non-local thermodynamic equilibrium (non-LTE) radiative transfer for the purposes of accurately retrieving temperatures and constituents was a frontier of active research. All infrared emissions measured by SABER (CO_2 (15 and 4.3 μm), O_3 (9.6 μm), H_2O (6.7 μm), OH (1.6 and 2.0 μm), NO (5.3 μm), and $O_2(^1\Delta$, 1.27 μm)) are from transitions that depart from local thermodynamic equilibrium in the mesosphere and lower thermosphere. Each of these emission features require extraordinarily complex modeling, at the molecular transition level, of collisions, radiative absorption and emission, and chemical excitation and energy transfer. A 4.3 μm CO_2 channel was included in SABER, taking the long view that it would eventually provide a pathway for retrieving CO_2 concentrations in the future. The SABER team were aware that Crutzen (1970) noted the mean free path of a 4.3 μm photon at 80 km was 200 m, implying that limb views of 4.3 μm radiance were unlikely to contain much information about the tangent layer, and hence, accurate, *operationally routine* retrievals of CO_2 would be very challenging. Eventually, daytime-only combined temperature and CO_2 retrievals were developed for SABER (Mertens, Russell et al., 2009; Rezac, Kutepov, et al., 2015). However, the primary SABER temperature data product, day and night, is derived using CO_2 concentrations provided by the Whole Atmosphere Community Climate Model (WACCM3) described by Garcia, Marsh, et al., 2007. WACCM3 continuously updates the CO_2 concentrations in accordance with the observed surface increase. This version of the SABER dataset is referred to as Version 2.07.

3. Algorithm Instability in SABER temperatures from 2020 to mid-2022

The first indication that there may be a problem with SABER temperatures for 2020 and onward came in developing the analyses reported recently by *Mlynczak, Hunt, et al*., (2022), who examined trends and changes in temperature and geopotential height measured by SABER from 2002 to 2021. Figure 1 shows the difference between the SABER Version 2.07 global annual mean temperatures in 2020 and 2009. We chose to compare these two years because they are both near a solar minimum, such that any impact of the solar cycle on the temperature difference is expected to be small.

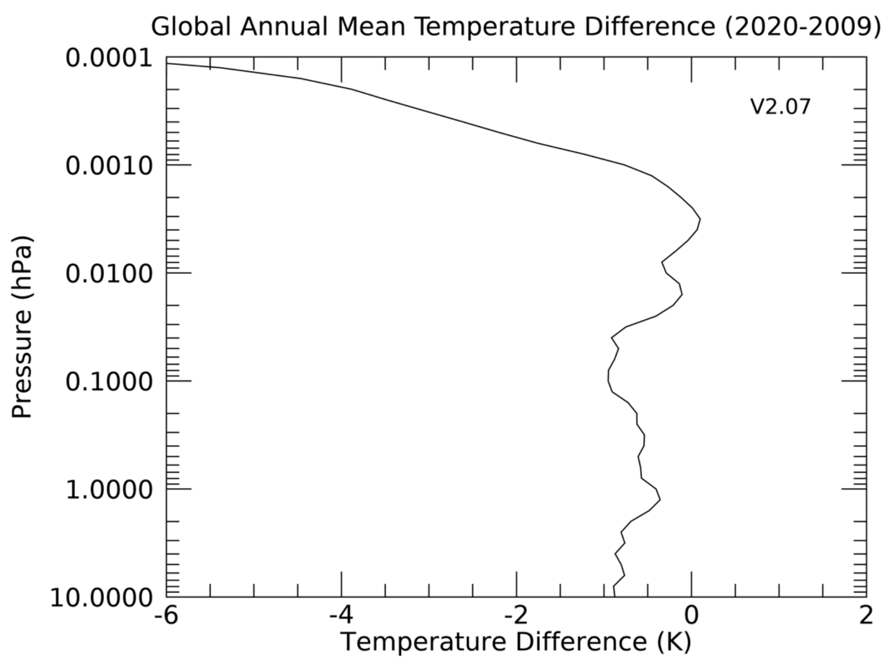

Figure 1. Difference (K) in SABER Version 2.07 global annual mean temperatures in 2020 and 2009. Note the rapidly increasing difference in temperature at pressures less than 4 x 10^{-3} hPa.

From 10 hPa (approximately 30 km altitude) to 0.01 hPa (approximately 80 km altitude) the temperature differences are between -0.1 K and -0.9 K. The expected difference in temperatures from 2009 to 2020 over this altitude range from increasing anthropogenic CO_2 is between -0.5 K and -0.6 K (Garcia, Yue et al., 2019; Mlynczak, Hunt, et al., 2022). However, at pressures less than 4 x 10^{-3} hPa (above 85 km) the data indicate the SABER temperature in 2020 is substantially colder than in 2009 by as much as 6 K. Solar cycle conditions, as indicated by the F10.7 index, were not markedly different in 2009 and 2020 (Mlynczak, Hunt, et al., 2022) as both years followed right after the occurrence of very quiet solar minimum conditions. The observed decreases in temperature of 2 K at 4 x 10^{-4} hPa and 6 K at 10^{-4} hPa from 2009 to 2020 correspond to the anticipated change from four or more decades of anthropogenic CO_2 increase based on trends reported by Mlynczak, Hunt, et al. (2022) and Garcia, Yue et al., (2019). The temperature differences, particularly at pressures less than 4 x 10^{-3} hPa are thus very difficult to explain based on solar activity or anthropogenic increases in CO_2. Note also that the rapid increase in the difference begins near 10^{-3} hPa, which is just the level where the CO_2 profiles from WACCM3 and WACCM4 begin to diverge noticeably, as shown below in Fig. 2. Finally, Mlynczak, Hunt, et al. (2022) also note that temperature trends of this magnitude are inconsistent with the expected sensitivity of the mesosphere and lower thermosphere to a doubling CO_2. The SABER team thus ruled out both anthropogenic CO_2 increase and a weaker solar minimum in 2019-2020 as the cause of the very large differences in temperatures at pressures less than 4 x 10^{-3} hPa between 2009 and 2020 shown in Figure 1.

In December 2019 the SABER team received several more years of CO_2 profiles from the WACCM team at NCAR to continue the operational processing of the day and night temperature data. The model output used for SABER data processing up to December 15, 2019 was obtained from WACCM3 (Version 3.5.48) simulations. To continue SABER processing into late December 2019 and beyond, additional WACCM output data extending into the 2020's was provided. WACCM Version 4 (WACCM4; Garcia et al., 2017) was the current version of the model in 2019, such that readily available output from this version was chosen for the continued operational processing of day and night SABER temperatures from December 16, 2019 onward. WACCM4 was chosen for the SABER operational data processing extension because it provided the best match to the WACCM3 CO_2 profiles in the stratosphere where the pressure registration using the (above mentioned) two-color technique occurs (Remsberg, Marshall et al., 2008). However, the WACCM4 ouput differed from WACCM3 (Version 3.5.48) in the rate of decrease of the CO_2 mixing ratio above ~85 km. This difference was due, in turn, to changes in the calculation of the vertical diffusivity due to parameterized gravity wave breaking, as described in Garcia, Lopez-Puertas, et al., 2014. This change led to larger vertical diffusivity in WACCM4 compared to WACCM3. The resulting differences in the CO_2 profiles were found to be the root cause of the rapid decrease in temperatures above ~85 km observed with SABER Version 2.07 temperatures shown in Figure 1. The WACCM4 CO_2 values are larger than those in WACCM3, and because of the 'inverse' relationship (discussed above) between temperature and CO_2 in the temperature retrieval algorithm, SABER temperatures from mid-December 2019 onward are markedly colder above 85 km.

Figure 2 shows the average monthly Version 2.07 CO_2 profiles for November 2019 and 2020 and their percent difference. The CO_2 concentrations at pressures less than 0.003 hPa are different by as much as 15% due to the change in the model version used in the SABER operational processing, from WACCM3 to WACCM4. The resulting SABER increase in CO_2 in the mesosphere and lower thermosphere is about 5% to 6% *per decade* (Yue, Russell, et al., 2015; Rezac, Kutepov, et al., 2015; Mlynczak, Hunt et al., 2022). Thus, the change in CO_2 introduced into the algorithm starting on December 16, 2019 was up to 30 times larger (at 0.0001 hPa) than expected from anthropogenic CO_2 increase. This discontinuity in the CO_2 profiles used in the Version 2.07 algorithm had a marked effect on the retrieved temperatures above ~ 85 km beginning in the second half of December 2019 until mid-2022, when they were understood and subsequently corrected.

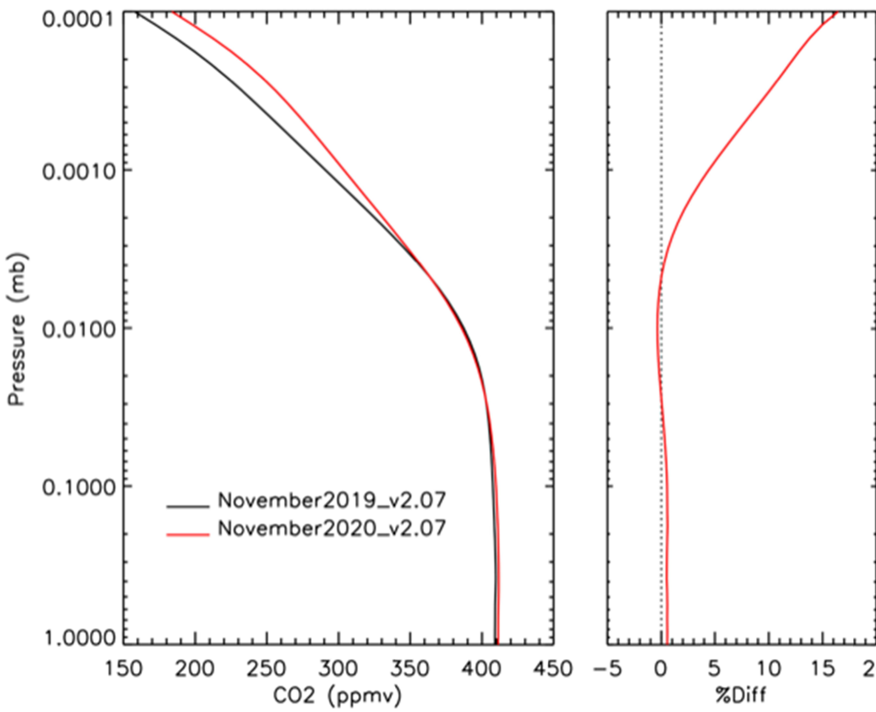

Figure 2. Monthly average CO_2 concentrations (ppmv) used in the operational retrieval of temperature (SABER Version 2.07) in November 2019 and November 2020 (left) and percentage difference (2020 minus 2019, right). This figure illustrates that for pressures less than 0.003 hPa (mb) up to 0.0001 hPa (mb), a change as large as 15 percent occurred in the concentration of CO_2 from 2019 to 2020.

After the algorithm instability was identified, the SABER and WACCM teams recovered the WACCM3 model output from December 15, 2019 onward that was consistent with the CO_2

used before December 15, 2019. The entire SABER dataset (all parameters, not just temperature) was reprocessed from December 16, 2019 and continues to the present day as all data products depend on temperature for their derivation. This new version, Version 2.08, has been publicly available since August 2022. Henceforth the naming conventions for SABER temperature data will be Version 2.07 for temperature data spanning January 2002 through December 15, 2019. Version 2.08 spans the period from December 16, 2022 onward. SABER Version 2.07 data after December 16, 2022 has been removed from the SABER data website and should not be used for scientific research henceforth.

Figure 3 shows the difference in Version 2.08 global annual mean temperatures in 2020 and the Version 2.07 global annual mean temperatures in 2009. The large temperature differences at pressures less than 4 x 10^{-3} hPa shown in Figure 1 are no longer present. The temperature differences at pressures greater than 4 x 10^{-3} are within the expected range for increasing CO_2 over 11 years and natural variability. Temperatures at lower pressures up to 10^{-4} hPa are up to 2 K colder in 2020 than 2009. Mlynczak, Hunt, et al. (2022) suggested that this could be a result of slightly lower solar irradiance in the Schumann-Runge absorption bands of molecular oxygen (175-200 nm) that play an important role in the heat budget of the lower thermosphere.

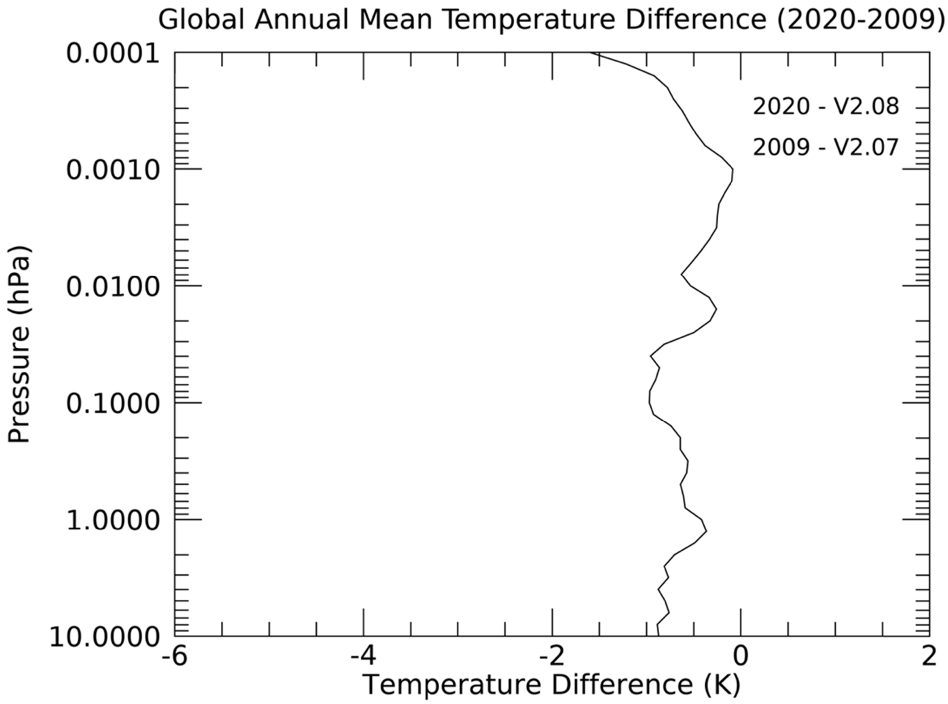

Figure 3. Difference in SABER Version 2.08 global annual mean temperatures in 2020 and Version 2.07 global annual mean temperatures in 2009. The large temperature differences shown in Figure 2 in 2020 for Version 2.07 are now absent.

4. Discussion and Summary

In this paper we have introduced the concept of a Geospace Data Record, a counterpart to the established Climate Data Record. Generating quality GDRs and CDRs is a meticulous and time-consuming process. As demonstrated above, unrecognized, or initially inconspicuous changes to the algorithm used to produce a long-term data record can promptly result in changes to the data time series that are larger than anticipated from real physical processes on decadal timescales. When constructing CDRs the emphasis has often been placed on examining and understanding the accuracy and stability over time of the instrument calibration. The SABER instrument calibration has been shown to be remarkably stable, primarily because of the decision made by the SABER team to focus on accurate calibration of the instrument from the beginning of its development (Mlynczak, Daniels, et al., 2020). The SABER experience has now shown that algorithm instability may introduce spurious behavior if undetected.

Algorithm instability in data products derived from satellites can also be induced by 'orbit instability' if the scientific algorithm contains terms that depend on satellite orbital parameters such as altitude or inclination. An example of orbit decay-induced algorithm instability was reported by Wentz and Schabel (1998) in tropospheric temperatures obtained by Microwave Sounding Unit (MSU) instruments. Wentz and Shabel showed that uncorrected effects of orbital decay on the satellites hosting the MSU instruments directly impacted the algorithm used to derive temperature and resulted in the MSU dataset exhibiting a cooling trend in tropospheric temperatures from 1979 to 1998 while other measurements showed the troposphere was warming. Prior to Wentz and Schabel's paper, the differences between MSU and other measurements were a source of controversy in the tropospheric climate community for some time. Wentz and Schabel demonstrated that when the orbit-decay induced effects were correctly accounted for, the MSU dataset exhibited a warming trend in troposphere temperatures consistent with other measurements and consistent with the anticipated global warming due to anthropogenic CO_2 increase.

Over next several decades, CDRs and GDRs will be developed from several different instruments, with potentially different measurement techniques, with different calibration accuracies, different calibration stabilities, and very likely, different algorithms requiring different inputs (e.g., spectroscopic databases). Each of these differences will add uncertainty to the accuracy of the trend derived from the combined long-term record. Lack of continuity and/or lack of measurement accuracy can render it nearly impossible to construct a long-term CDR or GDR with a scientifically (or economically) useful trend accuracy (e.g., Loeb, Wielicki et al., 2009). The tropospheric climate community is going to great lengths to achieve extremely high accuracy (and hence, extremely stable calibration) in the next generation of satellite-based climate missions with the Climate Absolute Radiance and Refractivity Observatory (CARREO) Pathfinder mission, the Traceable Radiometry Underpinning Terrestrial- and Helio-Studies (TRUTHS) mission, the LIBRA mission, and the Far-Infrared Outgoing Radiation Understanding and Monitoring (FORUM) mission (Shea, Fleming, et al., 2020; Fox, Kaiser-Weiss, et al., 2011; Zheng, Lu, et al., 2020; and Palchetti, Brindley, et al., 2020). These missions will enable construction of exceptionally accurate CDRs over decades. The field of geospace climate is now emerging as a forefront of scientific research and economic relevance. The geospace community can draw from the experience in the development of CDRs and tailor it to the requirements to produce accurate GDRs from future space and ground-based observations.

In this paper we have highlighted the issue of algorithm instability, as this is just one of the many issues that must be adequately considered in developing long term GDRs, as discussed by Mlynczak, Yue, et al. (2021). For the broad field of geospace science, accurately detecting and attributing long term change due to increasing anthropogenic CO_2 and to ongoing solar variability, assembling multiple accurate GDRs is essential. This is both an issue of scientific discovery and of economic and practical interest related to the longevity of space debris (Cnossen, 2022) that may have repercussions for the rapidly growing space economy.

As with the development of SABER that began over 30 years ago, future geospace measurement systems must now be designed with consideration of measurement accuracy and stability, in both the measurement itself and the algorithms that produce the data. The field of Space/Geospace climate is now emerging as a frontier of scientific inquiry and potential economic relevance. As with all such endeavors, the demonstrable quality of the data will determine the long-term quality and value of the science.

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Open Research

All SABER data used in this paper is available from the SABER project data server at https://saber.gats-inc.com/data.php

Additional data analyses and graphics were done using ENVI version 4.8 (Excelis Visual Information Solutions, Boulder, Colorado)

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Figure 1.

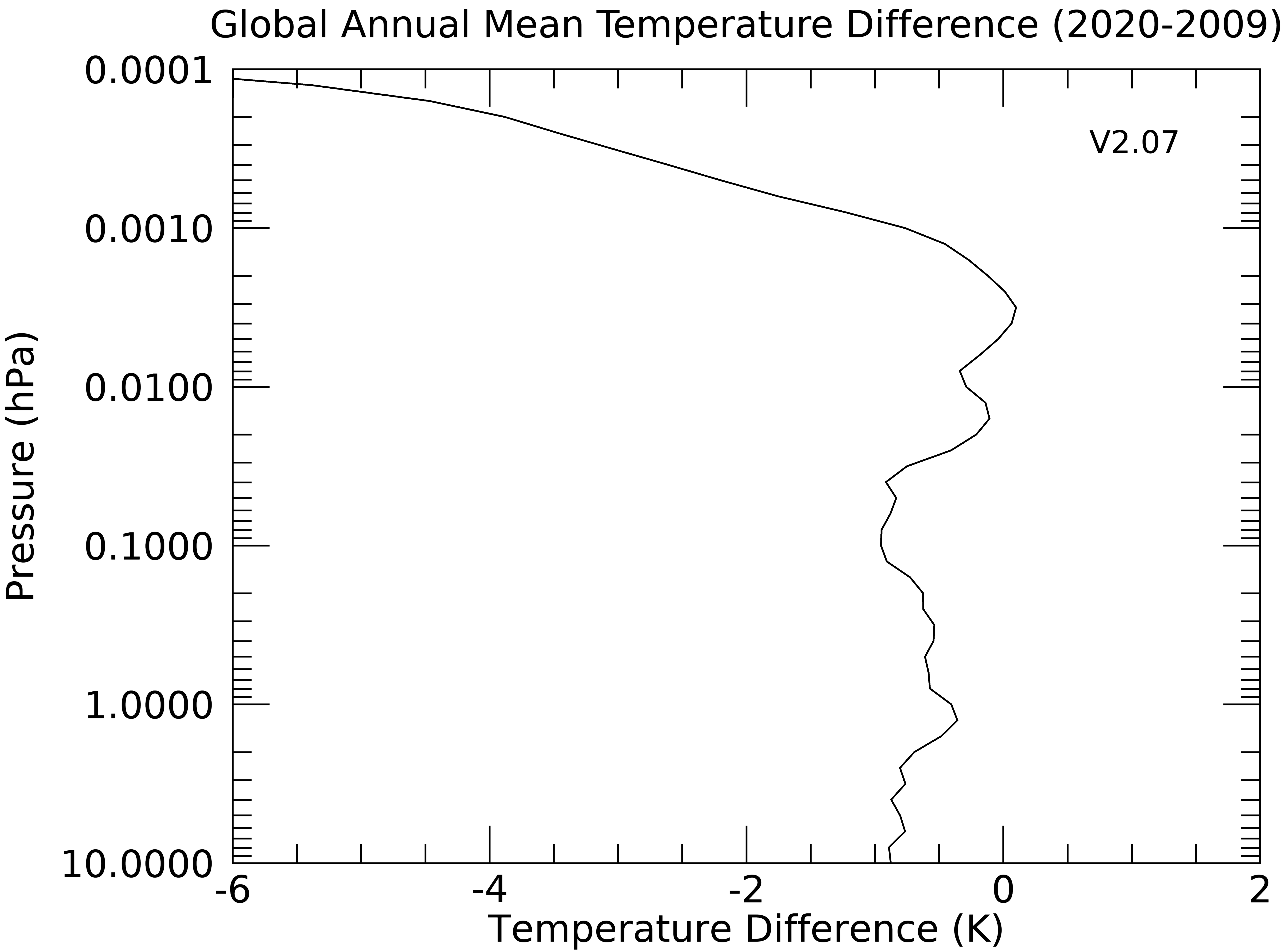
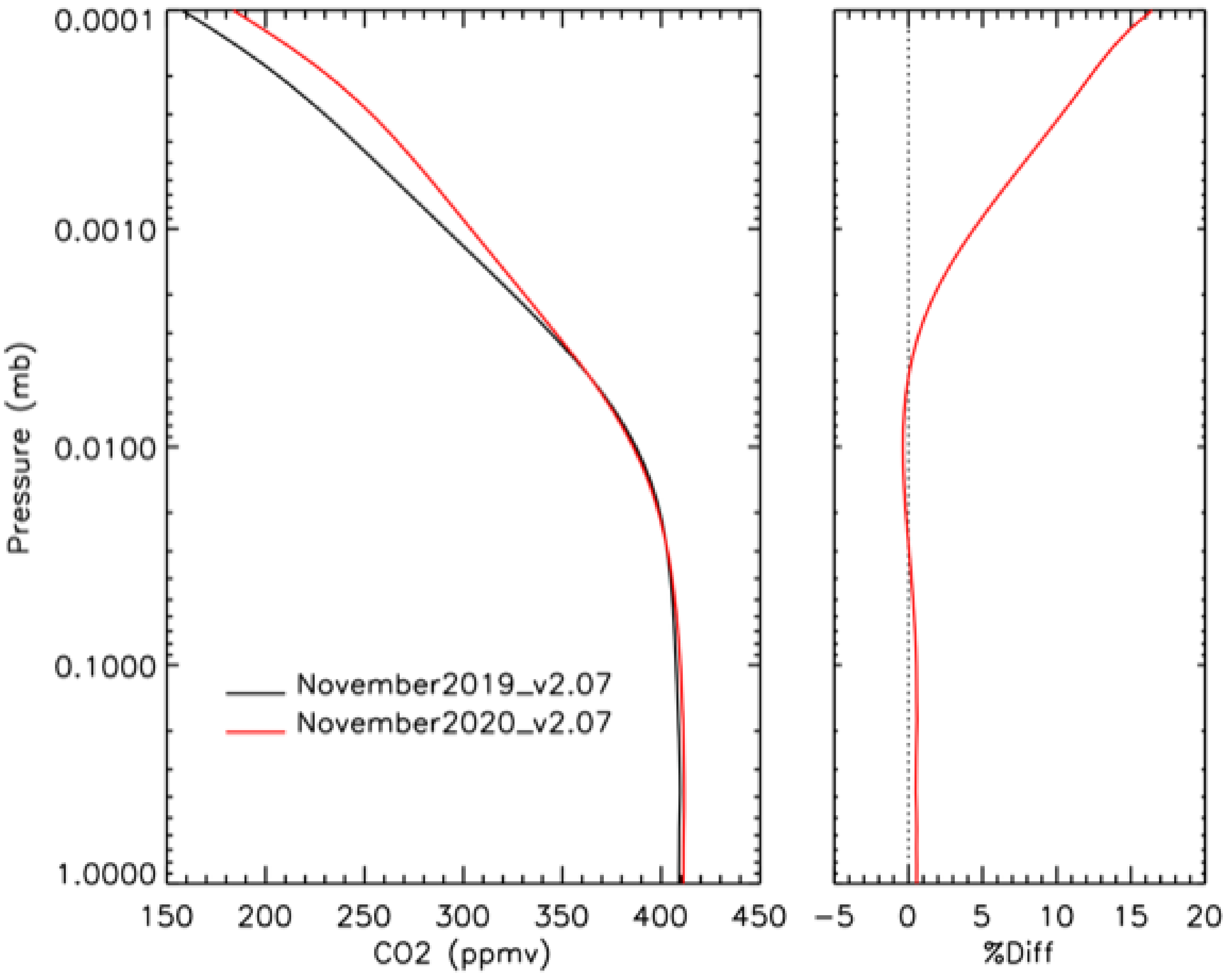
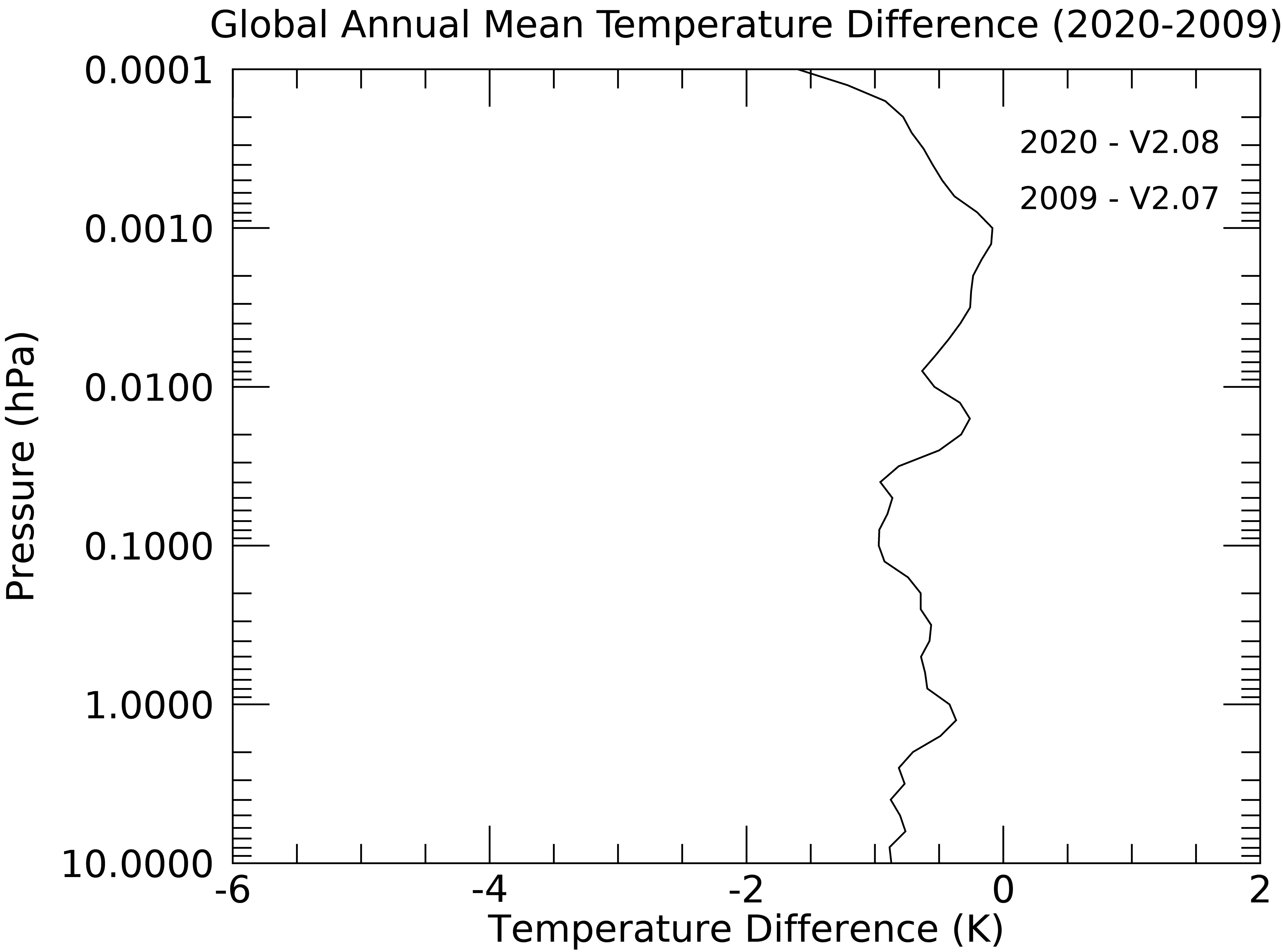

Global Annual Mean Temperature Difference (2020-2009)
V2.07
Pressure (hPa)
0.0001
0.0010
0.0100
0.1000
1.0000
10.0000
-6
-4
-2
0
2
Temperature Difference (K)

Figure 2.



0.0001
0.0010
0.0100
0.1000
1.0000
Pressure (mb)
150
200
250
300
350
400
450
CO2 (ppmv)
November2019_v2.07
November2020_v2.07
-5
0
5
10
15
20
%Diff

Figure 3.


Global Annual Mean Temperature Difference (2020-2009)
2020 - V2.08
2009 - V2.07
0.0001
0.0010
0.0100
0.1000
1.0000
10.0000
Pressure (hPa)
-6
-4
-2
0
2
Temperature Difference (K)