

Improving the Thermosphere Ionosphere in a Whole Atmosphere Model by Assimilating GOLD Disk Temperatures

F. I. Laskar¹, N. M. Pedatella², M. V. Codrescu³, R. W. Eastes¹, W. E. McClintock¹,

¹Laboratory for Atmospheric and Space Physics, University of Colorado, Boulder, CO, USA

²High Altitude Observatory, National Center for Atmospheric Research, Boulder, CO, USA

³Space Weather Prediction Center, NOAA, Boulder, CO, USA

Key Points:

- A new approach has been developed to assimilate GOLD T_{disk} in WACCMX which is validated using independent measurements.
- Analysis states of both the thermosphere and ionosphere show improved agreement with independent measurements.
- Results demonstrate a great potential of the GOLD T_{disk} data to improve understanding of the thermosphere ionosphere.

Abstract

Global-scale Observations of Limb and Disk (GOLD) disk measurements of far ultraviolet molecular nitrogen band emissions are used to retrieve column integrated disk temperatures (T_{disk}), which are representative of the lower-and-middle thermosphere. The present work develops a new approach to assimilate the T_{disk} in the Whole Atmosphere Community Climate Model with thermosphere-ionosphere eXtension (WACCMX) using the Data Assimilation Research Testbed (DART) ensemble adjustment Kalman filter. A total of 9 days of data during 1 to 9 November 2018 are assimilated. Analysis state variables such as thermospheric effective temperature (T_{eff}), ratio of atomic oxygen to molecular nitrogen column densities (O/N_2), and column electron content are compared with a control simulation that is only constrained up to ~ 50 km. It is observed that assimilation of the GOLD T_{disk} improves the analysis states when compared with the control simulation. The analysis states, particularly, T_{eff} , O/N_2 , and column electron contents are also compared with their measurement counterparts for the validation of the assimilation. T_{eff} and O/N_2 are compared with GOLD T_{disk} and O/N_2 . While, the Electron Column Density (ECD) from the analyses is compared with ground based Total Electron Content (TEC) measurements from Global Navigational Satellite System (GNSS) receivers. Root Mean Square Error (RMSE) improvements in T_{eff} and O/N_2 are about 12.8% and 13.2%, respectively. The RMSE improvement in analyses ECD is about 8% compared to control simulation.

Plain Language Summary

Understanding of the temperature and density variability of the thermosphere-ionosphere system is very important for satellite drag calculations and satellite communication. The thermosphere-ionosphere system is influenced by waves from the lower atmosphere and solar and geomagnetic forcing from above. For the characterization of this coupled system, realistic whole atmosphere ionosphere parameters are of great interest. The GOLD satellite mission provides daytime thermospheric temperature observations with unprecedented local time and spatial coverage. Including them with the lower and middle atmospheric observations in a whole atmosphere data assimilation system, we find that they improve the state of the thermosphere-ionosphere. This shows the promise of the GOLD disk temperatures in improving thermosphere-ionosphere states and their potential use to improve space weather forecast capabilities.

1 Introduction

Improvements in the satellite drag forecasts and satellite communication depend on a better understanding of the thermosphere-ionosphere (TI) system variability. Earth's TI system is coupled to the lower atmosphere by wave-dynamical forcing and to the solar and geomagnetic forcing from above. The lower atmospheric forcing also varies with location and time. Thus, for a better understanding of this coupled system, a global four dimensional dataset with good temporal and spatial resolution is needed. Satellite measurements from low-Earth orbit can provide good spatial coverage, but they lack local time coverage, unless a constellation of satellites is used. Ground based observations on the other hand have good local time coverage, but they are not available globally due to the significant fraction of the Earth that is covered by ocean. Moreover, the currently available whole atmosphere ionosphere thermosphere observations have data gaps at different altitudes and geographic locations. However, the currently available observations and state-of-the-art whole atmosphere model simulations can be combined in a data assimilation framework. Data assimilation combines observations with model forecasts to produce analysis states that can better estimate the current state of the TI system.

With time the whole atmosphere ionosphere thermosphere models are improving, and the TI system and lower atmosphere observations are increasing. Therefore, we are in a great stage to do a whole atmosphere data assimilation by combining the models and the observations. There is a long-history of lower atmosphere data assimilation (Rienecker et al., 2011; Gelaro et al., 2017; Hersbach et al., 2020), but the whole atmosphere system data assimilation is relatively new. There have been significant developments in the assimilation of thermosphere-ionosphere observations such as, neutral density (Ren & Lei, 2020; M. V. Codrescu et al., 2004; Matsuo et al., 2013; S. M. Codrescu et al., 2018; Sutton, 2018; Mehta et al., 2018), thermospheric temperature (Laskar, Pedatella, et al., 2021), thermospheric airglow irradiance (Cantrall et al., 2019), and electron content (Bust et al., 2004; Lee et al., 2012; Datta-Barua et al., 2013; Matsuo et al., 2013; Lin et al., 2015; Aa et al., 2016; Chen et al., 2016; Bust & Immel, 2020; Pedatella et al., 2020; He et al., 2020; Kodikara et al., 2021; Song et al., 2021; Forsythe et al., 2021). While these results were promising and showed that the assimilation of TI observations improves the model states, most were limited to using upper atmosphere only models or used limited thermospheric datasets from low-earth-orbit satellites or ionospheric only measurements or observing system simulation experiments. Furthermore, a majority of them have not

combined lower, middle, and upper atmosphere data in the assimilation. Also, the spatial and temporal coverage of thermospheric data available earlier were limited.

Temperature is one of the basic parameters in whole atmosphere models. Neutral temperature retrieved from Global-scale Observations of Limb and Disk (GOLD) disk measurements have increased the number of thermospheric observation dramatically, which enables a whole atmosphere data assimilation that can improve the specification of the TI system. Laskar, Pedatella, et al. (2021) performed a set of Observing System Simulation Experiments (OSSEs) to evaluate the impact of assimilating GOLD T_{disk} observations on thermospheric temperature and dynamics. They found that the OSSE that includes the GOLD T_{disk} improved the model temperature root mean square error (RMSE) and bias by 5% and 71% when compared with the forecast state, and the improvements are 20% and 94% when compared with lower atmosphere only assimilation. Laskar, Pedatella, et al. (2021) also found that the migrating diurnal tide (DW1) and local diurnal tide over Americas improve by about 8% and 17%, respectively, upon assimilation of GOLD disk temperature (T_{disk}) observations. In the current study we assimilate actual GOLD T_{disk} in a whole atmosphere data assimilation system and assess their impact on the thermosphere-ionosphere parameters by validating analysis states with their measurement counterparts.

2 Data, Models, and Methodology

The primary dataset used is the GOLD T_{disk} , which has been assimilated in the Whole Atmosphere Community Climate Model with thermosphere-ionosphere extension (WACCMX). In addition to T_{disk} , lower and middle atmosphere data have also been assimilated. For validation of the analysis states from the assimilation system, independent measurements of GOLD O/N₂ and Global Navigation Satellite System Total Electron Content (GNSS-TEC) are also used. Further details of these data and models are given below.

2.1 GOLD T_{disk}

GOLD observed the Earth's thermosphere in the far ultraviolet wavelengths for over 18.5 hours each day, from 0610 to 0040 Universal Time (UT) of the next day (Eastes et al., 2019, 2020; McClintock et al., 2020; Laskar et al., 2020). The primary GOLD ob-

servations are emission intensities in the far ultraviolet (FUV) range of 134.5 to 166.5 nm. Data for one full disk are available at every 30 minutes from 6-23 UT (Eastes et al., 2019, 2020; Laskar, Eastes, et al., 2021). The current investigation uses level 2 T_{disk} data (version 3) that are retrieved from 2×2 binned level-1C data, which are available in the GOLD web-page, <https://gold.cs.ucf.edu/> as ‘Level 2 - TDISK’. The retrieval algorithm is an improvement of the previously used methods for limb measurements (Aksnes et al., 2006; Krywonos et al., 2012).

The 2×2 binned data have a spatial resolution of $250\text{-km} \times 250\text{-km}$ near nadir. The GOLD daytime disk scans in N_2 Lyman-Birge-Hopfield (LBH) bands are used to retrieve T_{disk} data. Effective altitude and contribution function (CF) of the T_{disk} varies with solar zenith angle (SZA) and emission angle (EA). The SZA variation of the CF is well quantified (Laskar, Pedatella, et al., 2021) and thus is included in the present assimilation. However, the EA effects are not yet included in the assimilation. But, it has been observed that the EA does not impact the CF for EAs below 50° , so the T_{disk} data having $EA > 50^\circ$ are not included in this assimilation and analysis. This limit also restricts the latitude and longitude coverage, as shown in Figure 1, to about $\pm 50^\circ$ in latitude and about -10°W to -90°W in longitude. Also, for high SZA observations the signal to noise ratio (SNR) is low, which for the current V3 T_{disk} introduces a bias. Thus, the low SNR observations having $SZA > 65^\circ$ are not considered in the analysis and assimilation.

2.2 GOLD O/ N_2

GOLD disk measurements of OI-135.6 nm emission and N_2 -LBH bands in the $\sim 134\text{-}162$ nm wavelength range are used to retrieve the ratio of atomic oxygen to molecular nitrogen column densities ($\Sigma O / \Sigma N_2$) (Correira et al., 2020). For simplicity we use the notation O/ N_2 instead of $\Sigma O / \Sigma N_2$. The disk O/ N_2 has the same spatial and temporal coverage as that of the T_{disk} . O/ N_2 data are used here only for the comparison and validation of the analyses O/ N_2 . We use the 2×2 binned version 3 O/ N_2 data, named as ‘Level 2 - ON2’ in the GOLD data repository. Also, as the GOLD O/ N_2 is not optimized for auroral latitudes (Correira et al., 2020), the latitudes above $\pm 60^\circ$ are not used in the current analysis.

2.3 GNSS-TEC

The GNSS-TEC data used in this study are obtained from the madrigal database (<https://cedar.openmadrigal.org>). Madrigal TEC maps are derived from worldwide GNSS ground-based receivers. The vertical TEC data are available at 5 min temporal and 1° by 1° spatial bins. Details on the TEC retrieval algorithm can be found in Rideout and Coster (2006) and Vierinen et al. (2016). In the current study the TEC maps are averaged over 20 minutes centered at every UT hour to compare them with the analysis ECD from assimilation. The 20 minutes averaging is chosen to get enough satellite passes over a particular spatial grid.

2.4 WACCMX

The WACCMX version 2.1 is a whole atmosphere general circulation model extending from the surface to the upper thermosphere (~ 500 -700 km depending on solar activity) (Liu et al., 2018). WACCMX includes the chemical, dynamical, and physical processes that are necessary to model the lower, middle, and upper atmospheres. The thermosphere and ionosphere processes in WACCMX are similar to those in the NCAR Thermosphere-Ionosphere-Electrodynamics General Circulation Model (TIE-GCM), including the transport of O^+ and self-consistent electrodynamics as well as realistic solar and geomagnetic forcing. The model horizontal resolution is $1.9^\circ \times 2.5^\circ$ in latitude and longitude, and the vertical resolution is 0.25 scale heights above ~ 50 km.

2.5 SD-WACCMX

In this simulation the WACCMX horizontal winds and temperature are relaxed towards Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA2) (Gelaro et al., 2017; Rienecker et al., 2011), so we name it as Specified Dynamics WACCMX (SD-WACCMX). The relaxation or nudging to MERRA2 is up to 50 km altitude, and the model is free-running above this altitude (Marsh, 2011). The SD-WACCMX is used in this study as a control simulation. In addition to MERRA2, SD-WACCMX simulations (often referred here as SD-EXP) also use operational solar F10.7 cm flux and geomagnetic Kp index for forcing and thus they can be used as a control simulation for the assessment of the data assimilation states.

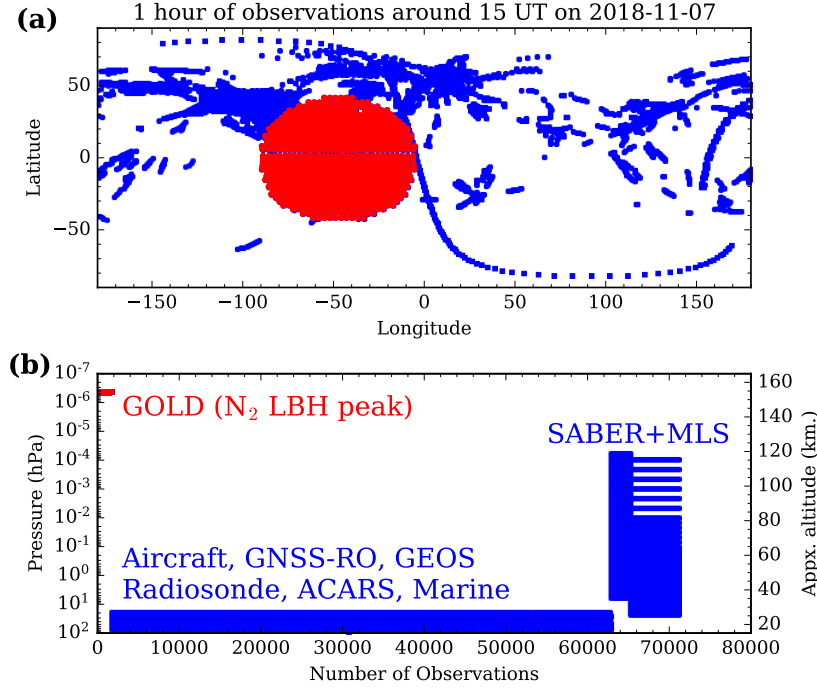


Figure 1. Geo-locations (a), altitude or pressure and number of observations (b) that are assimilated successfully during a representative hour on a particular day are shown. The red points show the GOLD observations and blue points are the rest of the observations, which we term as lower atmosphere observations including SABER and MLS.

2.6 WACCMX+DART

The data assimilation capability in WACCMX was initially implemented by Pedatella et al. (2018) using DART (J. Anderson et al., 2009), which uses the ensemble adjustment Kalman filter (J. L. Anderson, 2001). In the present work we assimilate lower and middle atmosphere as well as thermosphere observations in the WACCMX+DART. The lower atmosphere measurements include conventional meteorological observations (i.e., temperatures and winds from aircraft, radiosonde measurements, etc.), as well as GNSS radio occultation refractivity. Assimilation of these observations improves specifications of the troposphere-stratosphere globally, which is important for the studies of the vertical coupling of waves from lower-atmosphere to the thermosphere (Wang et al., 2011; Pedatella et al., 2014; McCormack et al., 2017; Pedatella et al., 2018).

In addition to lower altitude observations, middle atmosphere temperatures from Sounding of the Atmosphere using Broadband Emission Radiometry (SABER) instru-

ment on the Thermosphere Ionosphere Mesosphere Energetics and Dynamics (TIMED) satellite and Aura Microwave Limb Sounder (Aura-MLS) are also used. Altitude coverage of temperature profiles extends from stratosphere to mesosphere-lower-thermosphere (MLT) altitudes (~ 15 - 105 km for TIMED-SABER and ~ 15 - 90 km for Aura-MLS). The latitude coverage of TIMED-SABER retrieved temperature alternates between 83°S - 52°N (south viewing mode) and 83°N - 52°S (north-viewing mode) (Remsberg et al., 2008). We performed 9 days (1 to 9 November 2018) of data assimilation, during which TIMED-SABER was in the north-viewing mode on 1 November only. From 2 to 9 November it was in the south viewing mode. While for the Aura-MLS it varies from 82°S - 82°N (Schwartz et al., 2008). Though Aura-MLS and TIMED-SABER temperatures are middle atmospheric observations, for simplicity we refer to them here as part of lower atmosphere observations. Assimilation of these data has previously been demonstrated to improve specification of the MLT state and dynamics (Pedatella et al., 2014; McCormack et al., 2017; Laskar et al., 2019).

In addition to lower atmosphere observations, GOLD T_{disk} are used in the whole atmosphere assimilation. As the thermospheric dynamics can change fast in response to changes in forcing conditions, we use a 1 hour assimilation frequency. Additionally, Pedatella et al. (2020) have shown that using a 1 hr data assimilation cycle and removal of second-order divergence damping in WACCMX+DART significantly improves tidal amplitudes, which were previously found to be too small (Pedatella et al., 2018). Also, the lower atmosphere analysis states in WACCMX+DART agree well with other lower atmospheric assimilations, for example, MERRA2 (McCormack et al., 2021).

Figure 1 shows the locations (in a) and altitude or pressure vs. number of observations (in b) that are assimilated successfully during a representative hour on a particular day. The red points show the GOLD observations and blue points are the rest of the observations, which we term as lower atmosphere observations, including TIMED-SABER and Aura-MLS. Note that the peak altitude of the N_2 -LBH emission is shown here as a representative altitude of about 150 km, but in the assimilation the impact of T_{disk} is distributed over altitudes based on the SZA dependent CF (Laskar, Pedatella, et al., 2021). One can see that about 70000 observations per hour are assimilated. On an average about 1.5 million observations per day are assimilated. The simulations used in this study are listed in Table 1. The SD-WACCMX is used in this study as the control simulation.

Experiment	Observations Assimilated	Nudging Used	Model States Updated
SD-EXP (SD-WACCMX, Control Expt.)	N/A	MERRA2 U, V, T up to 50 km	N/A
DA-EXP1 (WACCMX +DART E1)	Meteorological, Aura-MLS-T, SABER-T, GOLD-T _{disk}	N/A	T
DA-EXP2 (WACCMX +DART E2)	Same as DA EXP1	N/A	T, O, O ₂ , O ⁺

Table 1. WACCMX simulation and data assimilation experiments used in this study are listed. U, V, T, N/A, SD, and DA stands for zonal wind, meridional wind, temperature, Not Applicable, Specified Dynamics, and Data Assimilation, respectively. Also, O, O₂, and O⁺ refers to the mass mixing ratio of atomic oxygen, molecular oxygen, oxygen ion, respectively. The short forms of the experiments are presented in bold.

We have performed two WACCMX+DART assimilations. One that assimilates lower atmosphere and GOLD T_{disk} observations and the direct impact of T_{disk} has been restricted only to the model temperature, referred to as DA-EXP1 in Table 1. The second experiment assimilates the same observations as the first experiment but the T_{disk} observations directly impact the model T, O, O₂, and O⁺, referred to as DA-EXP2 in Table 1. We used 40 ensemble members in the assimilation. In order to achieve sufficient spread in the ensemble members, we used a gaussian distribution of solar and geomagnetic forcing parameters with mean as the actual value with standard deviations of 15 sfu for F10.7 cm flux and 1 for Kp index. We reset any F10.7 value less than 60 sfu to 60 sfu and any negative Kp to 0. The forcing perturbations for a particular ensemble remains same for all the days. To avoid artifacts arising from initial ensemble members the spinup duration for the two assimilation runs are about 2 weeks.

3 Results

In order to assess and validate the performance of the assimilation we compare the ensemble averaged analysis states to their measurement counterparts. For example, effective temperature (T_{eff}) from model simulation is compared with GOLD T_{disk} ; O/N_2 is compared with GOLD O/N_2 ; and Electron Column Density (ECD) is compared with the GNSS-TEC. Note that T_{eff} here refers to the vertically integrated GOLD equivalent temperature that is calculated by integrating the model temperature profile weighted by the SZA dependent CFs. Also, the ECD is similar to TEC, but the column integration is only to the topmost layer of WACCMX, which is about 480 km for the current case. Figure 2 shows a comparison of the local time and latitude variation of the GOLD T_{disk} with T_{eff} from ensemble averaged states of the DA-EXP1 (DA-EXP1 T_{eff}) and SD-WACCMX (SD-EXP T_{eff}) for 2 different days. The latitudes and local times are restricted to only those locations and times where GOLD T_{disk} is being assimilated. Beyond those local time and latitudes GOLD data are available but we are not using them in the assimilation as explained in Sections 2.1 and 2.2. Note that in this figure only a representative longitude of $48^\circ W$ is shown, which is close to the sub-satellite point of GOLD.

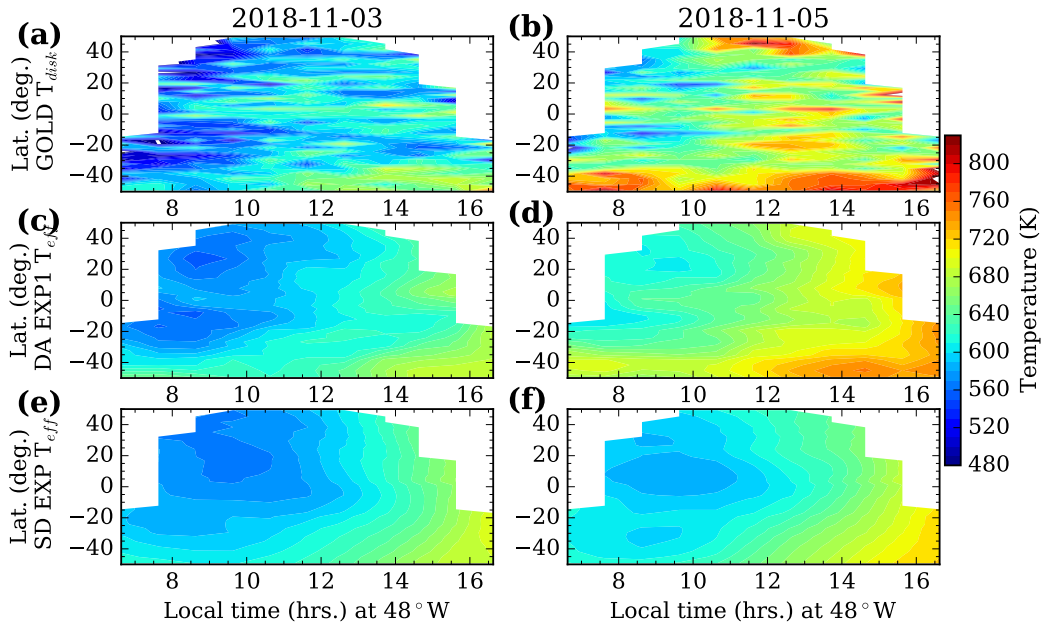


Figure 2. Local time and latitude variation of the GOLD T_{disk} compared with T_{eff} from DA-EXP1 (DA-EXP1 T_{eff}) and SD-WACCMX (SD-EXP T_{eff}).

It can be noted from Figure 2 that the broad variations between T_{disk} and DA-EXP1 T_{eff} are similar on both the days. On 5th November 2018 there was a moderate geomagnetic storm for which the average temperature is more than 100 K higher than 3rd November 2018. Moreover, the morning temperatures are relatively warmer, particularly between 40° and 50°S. These variations of the GOLD T_{disk} during geomagnetic events have been reported and discussed in Laskar, Eastes, et al. (2021). On both days the small scale local time features in T_{disk} can also be seen in DA-EXP1 T_{eff} , but they are absent in SD-EXP T_{eff} . This suggests that the data assimilation is driving the model temperature in the right direction. Quantitative estimate of the differences between them are given later. Note that since both the assimilation experiments updated the temperature directly at every assimilation step, the T_{eff} are nearly the same for both cases. So, the T_{eff} for only the DA-EXP1 is shown here.

The variation in temperature also changes other states by altering the model dynamics. Therefore assimilation of T_{disk} can also impact the O/N₂ ratio, which is another primary dataset from the GOLD. Figure 3 shows a comparison of GOLD O/N₂ with the O/N₂ from data assimilation and control simulation experiments, for the same 2 days shown in Figure 2. Unlike Figure 2, here the latitude range is extended to 60°N/S, as the GOLD O/N₂ are valid for those latitudes. We compare O/N₂ from the DA-EXP1 (c and d), DA-EXP2 (e and f), and SD-EXP (g and h) with the GOLD O/N₂ (a and b). Note that the GOLD O/N₂ observations have not been assimilated in any of the experiments. In the DA-EXP2 the GOLD T_{disk} observations also directly update the O, O₂, and O⁺ mass mixing ratios in addition to temperature. The direct updating of these quantities impacts the neutral composition and ionosphere at every assimilation step and thus they are expected to compare better than the indirectly updated states. It can be observed from Figure 3 that the broad variations in O/N₂ agree well between GOLD O/N₂ and the two assimilation experiments. Though interhemispheric features in SD-EXP, the assimilation experiments, and the observations match well there are clear differences in finer structures between them. For the quiet-day of 3rd November the two assimilation experiments show better agreement with GOLD O/N₂ compared to the SD-EXP O/N₂. The highest discrepancy in O/N₂ can be seen on the storm day (right panel) where the Northern higher-latitude depletion in the GOLD O/N₂ is nearly absent in SD-EXP and is weak in the two assimilation runs.

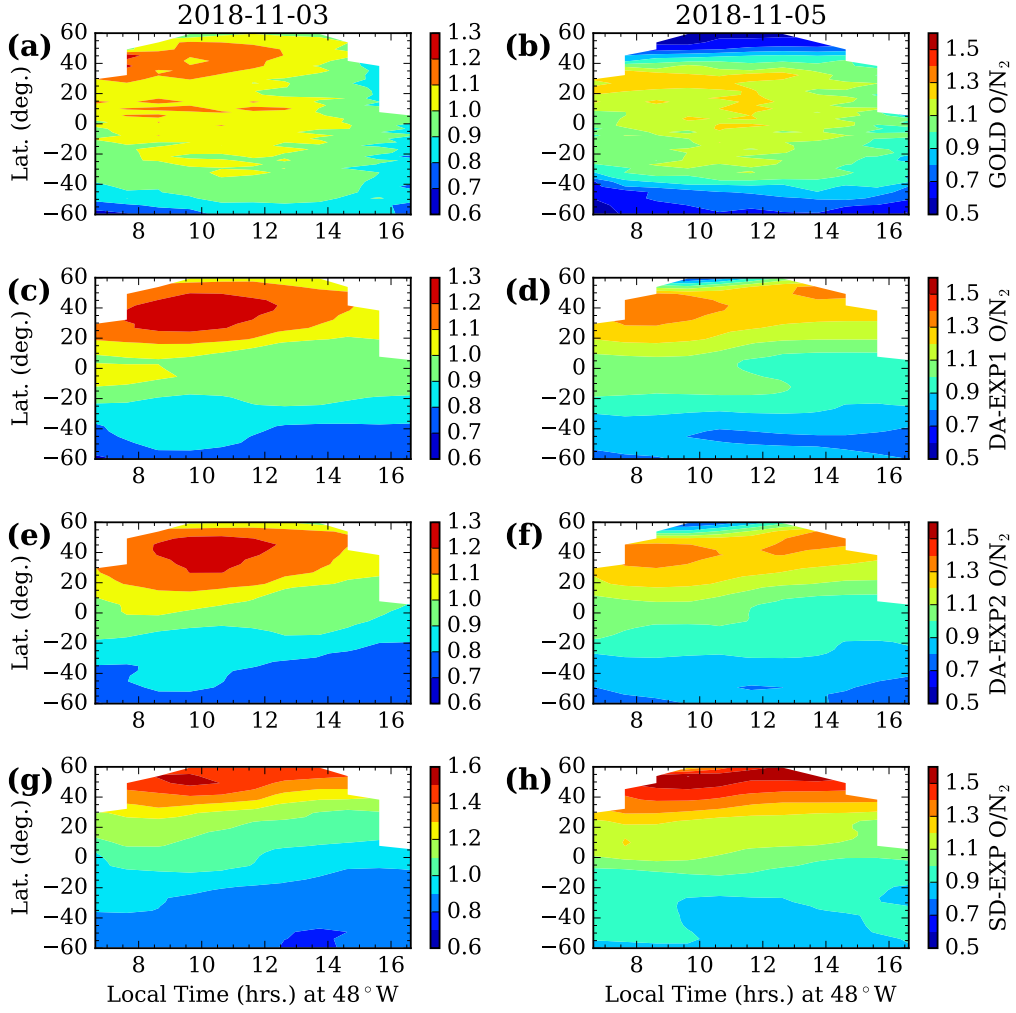


Figure 3. Same as Figure 2 but for the column integrated O/N_2 ratio. In addition to the DA-EXP1 the DA-EXP2 O/N_2 is also shown in (e and f).

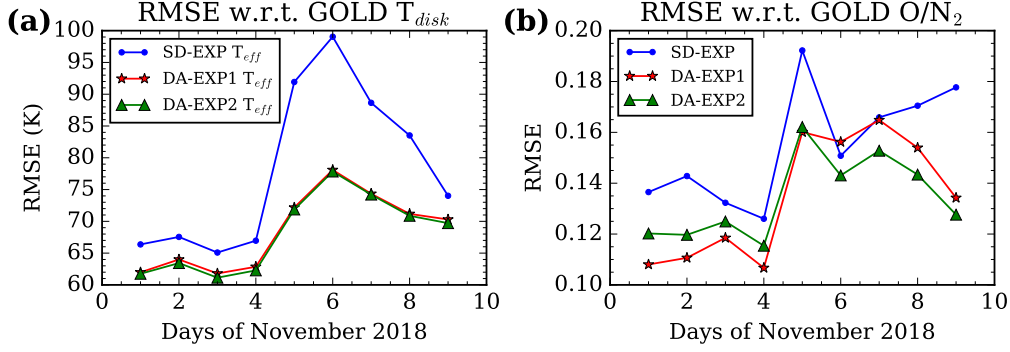


Figure 4. The RMSEs in DA-EXP1 T_{eff} and DA-EXP2 T_{eff} with respect to GOLD T_{disk} are shown in (a) and similar RMSEs in O/N_2 are shown in (b). Note that the temperature RMSEs in the two data assimilation runs, are clearly smaller than the SD-EXP. Also, the average O/N_2 RMSEs are better for the two assimilation runs compared to the SD-EXP.

For a quantitative estimation of the above observed differences between actual measurements and their data assimilation equivalents we calculate the Root Mean Square Error (RMSE). The RMSE in SD-EXP T_{eff} , DA-EXP1 T_{eff} , and DA-EXP2 T_{eff} with respect to GOLD T_{disk} are shown in Figure 4(a) for all the 9 days. The RMSE for each day is calculated over the whole disk and local time range as shown in Figure 2 for temperature and Figure 3 for O/N_2 . Note that the temperature RMSEs in the two data assimilation runs are clearly smaller than the SD-EXP. Also, the temperature RMSE for the two assimilation runs are almost same, which is expected as both the assimilations updated model temperature directly. The RMSEs in O/N_2 are shown in Figure 4(b). The average O/N_2 RMSEs are better for the two assimilation runs compared with the SD-EXP. The pre-storm RMSEs are smaller compared with storm onset and recovery phase. Average RMSE improvements in effective temperature and O/N_2 compared to the SD-EXP are about 12.8% and 13.2%, respectively. The improvements of pre-storm RMSE in T_{disk} and O/N_2 are about 6.4% and 11.3% while during the storm they were about 18.8% and 11.5%, respectively.

For a more robust diagnosis of the relationship between SD-EXP T_{eff} , DA-EXP1 T_{eff} , and DA-EXP2 T_{eff} with respect to GOLD T_{disk} for all the available latitudes, longitudes in the disk scans between 10 to 20 UT during 1 to 9 November 2018 we make scatter diagrams as shown in Figure 5, where the red color represents high density points.

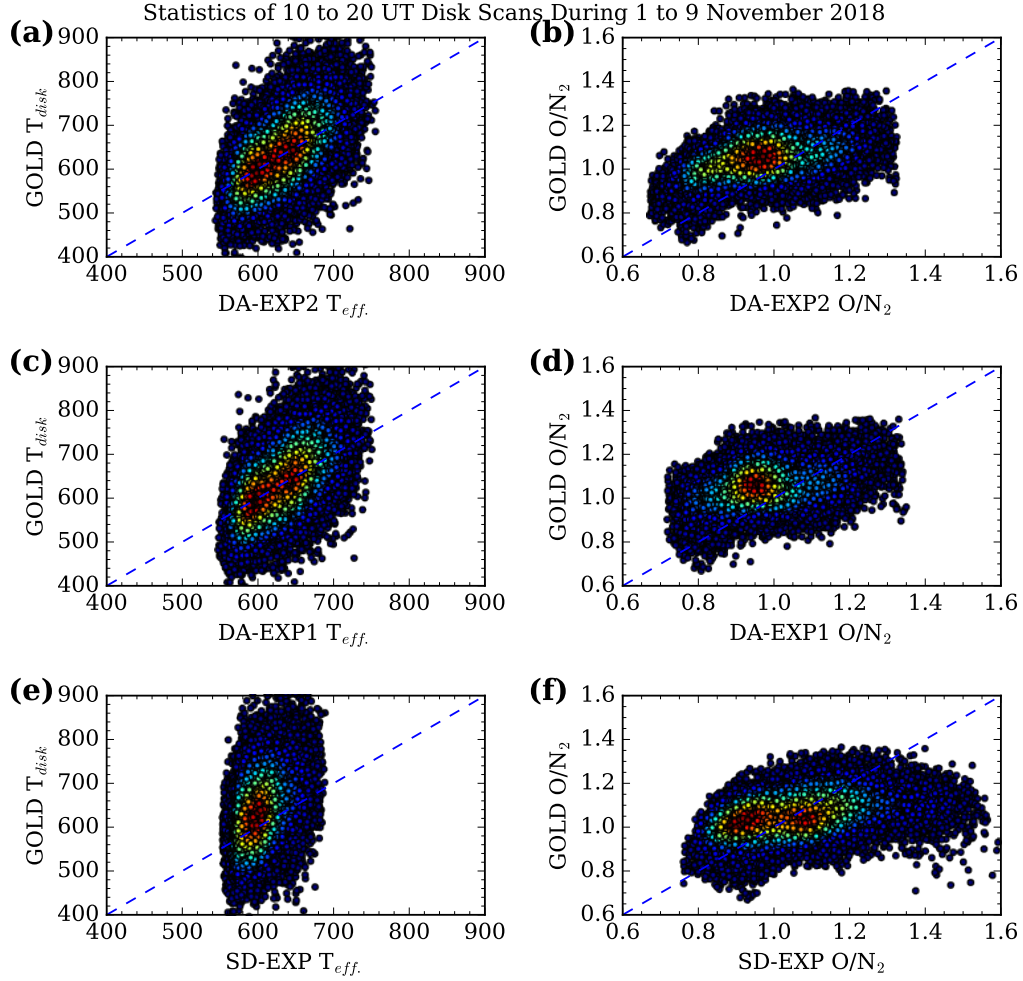


Figure 5. Scatter diagram of the GOLD T_{disk} and O/N_2 compared to their DA-EXP2, DA-EXP1, and SD-EXP equivalents are shown. For this analysis all the disk scans between 10 to 20 UT during 1 to 9 Nov. 2018 are used. The red regions in the scatter diagram represents highest density points. For the GOLD vs. DA-EXP2 the highest density points distribute around the linear 45° slope line, particularly for the temperature. The comparison w.r.t. SD-EXP for both temperature and O/N_2 , on the other hand, is not so good.

From these scatter plots it can be seen that the majority of the T_{disk} vs. DA-EXP2 T_{eff} points (in a) fall just over the linear correlation straight line with slope 45° . But, for the T_{disk} vs. SD-EXP T_{eff} (in e) comparison, the highest density observations (red points) deviate away from the linear fit with 45° slope. Note that here also, only those observations are shown that fall within the 50° EA and 65° SZA limits. As the GOLD T_{disk} has higher spread compared to DA-EXP2 T_{eff} , DA-EXP1 T_{eff} , and SD-EXP T_{eff} the shape of the scatter plot is elongated towards the T_{disk} axis (in a, c, and e). Similar to temperature, the O/N₂ scatter diagrams are shown in Figure 5(b, d, and f) but the EA and SZA restrictions are not applied here. Here also, the agreement of GOLD O/N₂ with DA-EXP2 O/N₂ (in b) is better compared with the GOLD vs. SD-EXP O/N₂ (in f). Though, the agreement for GOLD vs. DA-EXP2 O/N₂ is less than that of T_{disk} vs. DA-EXP2 T_{eff} , but there is significant improvement when compared with GOLD vs. SD-EXP O/N₂. The distribution of points in the GOLD T_{disk} vs. DA-EXP1 T_{eff} and GOLD T_{disk} vs. DA-EXP2 T_{eff} is nearly identical because the temperature was updated directly in both the assimilations. However, the distributions in O/N₂ in Figure 5(b and d) are significantly different. The O/N₂ scatter diagram for the GOLD vs. DA-EXP1 is better than the GOLD vs. SD-EXP but not as good as compared to GOLD vs. DA-EXP2.

The improvements in the O/N₂ motivated us to analyze the electron content derived from the assimilations and compare them with the independent measurements of GNSS-TEC. Figure 6 shows a latitude vs. day-to-day variation of ECD in SD-EXP (a), DA-EXP1 (b), DA-EXP2 (c), and GNSS-TEC (d) centered at around 60° W ($\pm 5^\circ$) longitude. This spatial bin has been chosen due to the greater availability of GNSS data in this region. As mentioned in section 2.3, the GNSS-TEC data are averaged over 20 minutes duration centered at every hour. Note that even with the 20 minute averaging, there are missing data, specifically between 20° and 40° N. This figure shows that the magnitudes of electron densities and the shape and temporal variability of Equatorial Ionization Anomaly (EIA) in DA-EXP2 has better agreement with GNSS-TEC compared to the DA-EXP1 and SD-EXP. Particularly, the northern mid-latitude enhanced DA-EXP2 ECDs are in better agreement with GNSS-TEC. Though there are improvements in DA-EXP2, the EIA latitude extent and hemispheric asymmetries are not yet well reproduced in the assimilations. This could be due to the fact that the temperature variability cannot fully reflect the changes in the ionosphere as the ionosphere is also influ-

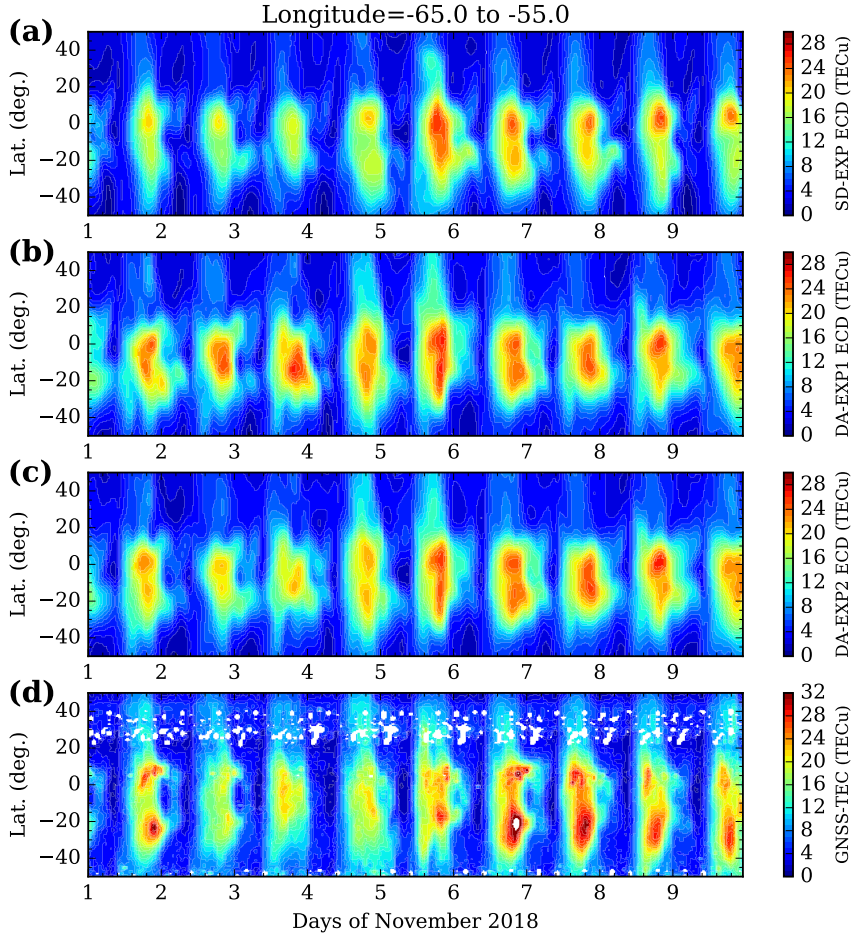


Figure 6. Latitude and day-to-day variability of SD-EXP ECD (a), DA-EXP1 ECD (b), DA-EXP2 ECD (c), and GNSS-TEC (d) averaged over 55°W to 65°W longitude.

enced by neutral and ionospheric composition changes. We expect to have better agreement in the future when the GOLD O/N₂ and other ionospheric dataset are assimilated in addition to the T_{disk} .

For a qualitative assessment of the improvements seen in the ionospheric electron content, a comparison between SD-ECD (green), DA-EXP1 ECD (cyan), DA-EXP2 ECD (red), and GNSS-TEC (blue) for a limited spatial region is shown in Figure 7(a). Also, the RMSE (in Figure 7b) and bias (in Figure 7c) with respect to GNSS-TEC are also shown. The DA-EXP2 ECD has better agreement with GNSS-TEC as can be inferred from the smaller values of the RMSE and bias. Some of the local time variabilities also have bet-

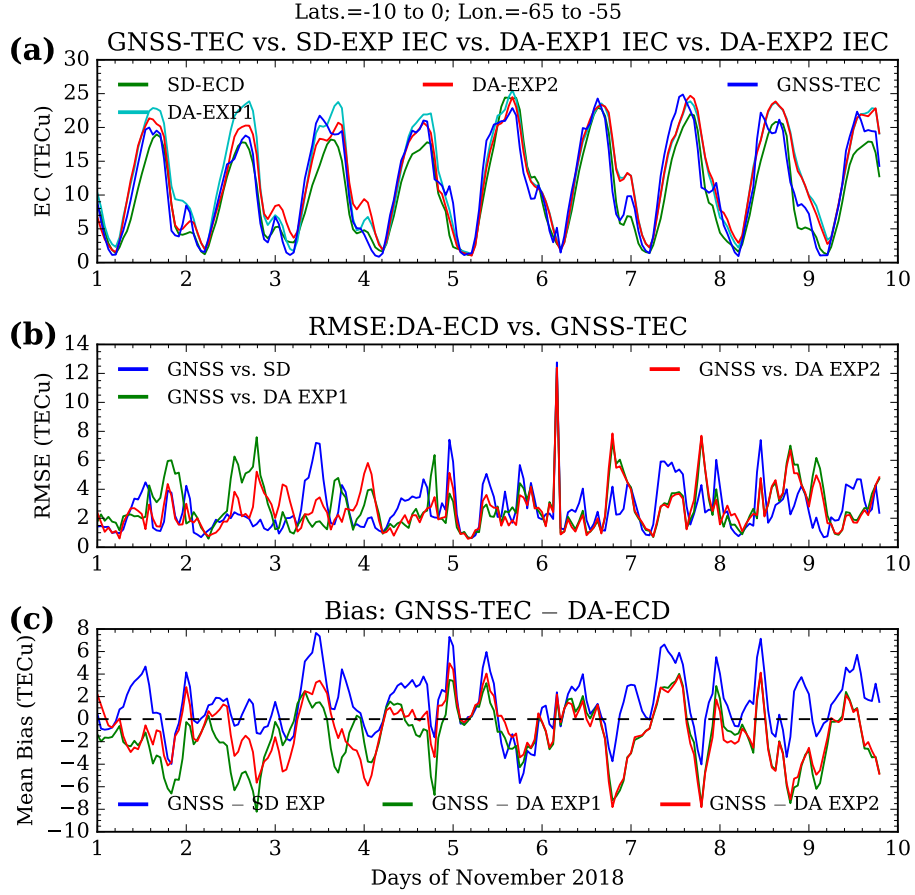


Figure 7. (a) Comparison of the SD-EXP ECD (green), DA-EXP1 ECD (cyan), DA-EXP2 ECD (red), and GNSS-TEC (blue) which are averaged over 10°S to 0°N and 55°W to 65°W . (b) RMSEs in GNSS-TEC vs. SD-EXP ECD (blue), GNSS-TEC vs. DA-EXP1 ECD (green), and GNSS-TEC vs. DA-EXP2 ECD (red). (c) Mean bias in GNSS-TEC vs. SD-EXP ECD (blue), GNSS-TEC vs. DA-EXP1 ECD (green), and GNSS-TEC vs. DA-EXP2 ECD (red) are shown.

ter agreement with DA-EXP2. For example, the two-peak structures in daytime GNSS-TEC on days 1, 3, 4, 5, and 9 are better reproduced in the DA-EXP2 ECD. Also, the broader shape of the local time variability in GNSS-TEC match better with DA-EXP2 ECD as can be seen on most days in Figure 7(a). Most of the higher RMSEs in DA occur during night-time sector, where GOLD T_{disk} observations are not available. The purpose of this comparison is to demonstrate that the ionosphere is also improved upon assimilation of GOLD T_{disk} . From Figure 7(c) it can be noted that the mean bias is also lower for the DA-EXP2 ECD. A quantitative estimate of the differences, that varies with latitude and time, are given below.

In Figure 3 we show that the GOLD O/N_2 has latitudinal differences from the DA O/N_2 . Also, we have seen in Figure 6 that the agreement between DA-EXP2 ECD and GNSS-TEC varies with latitude. To investigate these latitudinal differences in TEC we have calculated the RMSE and mean bias at every 10 degree latitude bin during the 9 days. The RMSE and mean bias in electron contents from SD-EXP, DA-EXP1, and DA-EXP2 with respect to GNSS TEC are shown in Figure 8. One can note that the lowest values of the RMSE and bias are observed for the DA-EXP2, the red lines marked with stars. The RMSE and bias at every latitude bin is calculated from all the $24 \times 9 = 216$ hours of data. The percentage improvements in RMSE for DA-EXP1 ECD and DA-EXP2 ECD with respect to GNSS-TEC are about 3% and 8%, respectively. The 9 day average mean biases with respect to GNSS-TEC for the SD-EXP, DA-EXP1, and DA-EXP2 are about 1.9, 0.5, and 0.8 TECu, respectively. Though the latitudinal average of the mean biases is slightly smaller for the DA-EXP1 compared to DA-EXP2, it is clear that the biases are smaller for both the assimilations compared to SD-EXP. Also, the mean bias is positive at higher latitudes ($> 30^\circ$) as seen in Figure 8(b). Since the O/N_2 and TEC vary in proportion, the lower O/N_2 (from GOLD as shown in Figure 3(b)) at the higher latitudes compared to SD and DA experiments produce the positive mean biases in TEC. These results further emphasize that the DA-EXP2 – where in addition to temperature the O, O^+ , and O_2 mixing ratios are updated directly – improves the thermosphere and ionosphere. Overall, it can be observed that the RMSEs are lower in the Northern hemisphere compared to the Southern hemisphere, which suggests that the Northern hemispheric variabilities are better reproduced in the assimilation.

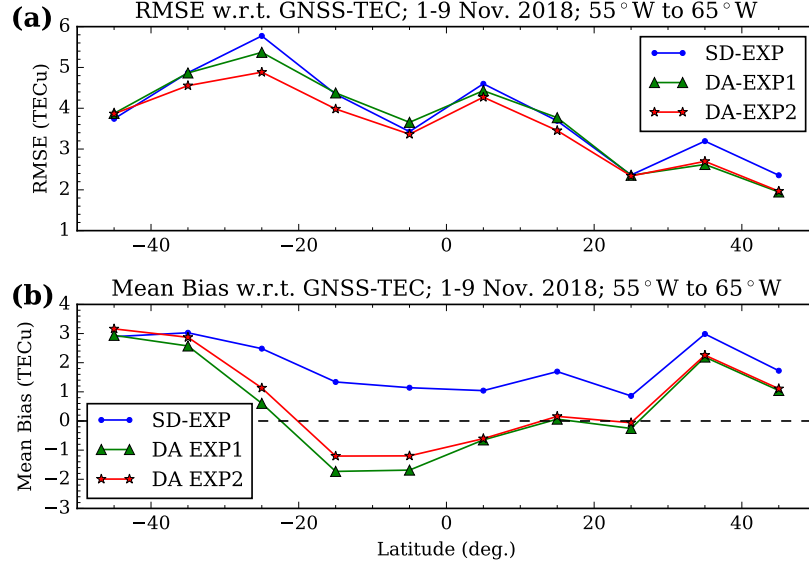


Figure 8. Latitudinal variability of RMSE (a) and mean bias (b) for SD-EXP (blue), DA-EXP1 (green), and DA-EXP2 (red) with respect to GNSS-TEC during 1-9 Nov. 2018 are shown. Clearly, for the DA-EXP2 the RMSE is smaller compared to other two cases and bias is closer to zero.

4 Conclusions

An investigation of the impact of GOLD T_{disk} assimilation on thermosphere-ionosphere states is carried out using WACCMX+DART. The salient results of this investigation are:

1. GOLD T_{disk} assimilation analysis states of the thermosphere-ionosphere show better agreement with independent measurements than the control simulation.
2. The GOLD T_{disk} and O/N_2 compare better with the WACCMX+DART effective temperature and O/N_2 when compared with equivalent parameters from SD-WACCMX.
3. The RMSE improvements in analyses effective temperature and O/N_2 , when compared to GOLD measurements, are about 12.8% and 13.2%, respectively.
4. The RMSE between GNSS-TEC and analysis electron column density (ECD) is better compared to that between GNSS-TEC and SD-WACCMX ECD. The improvement in this is about 8% for the assimilation that updates the O, O^+ , and O_2 densities in addition to temperature.

These results indicate that the GOLD observations of the thermospheric temperature has a great potential to improve the operational and short term forecast of the thermosphere-ionosphere system.

Acknowledgments

This research was supported by NASA Contract 80GSFC18C0061 to the University of Colorado, Boulder. This material is also based upon work supported by the National Center for Atmospheric Research (NCAR), which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977. Computing and data storage resources, including the Cheyenne supercomputer (<https://doi.org/10.5065/D6RX99HX>), were provided by the Computational and Information Systems Laboratory (CISL) at NCAR. WACCMX is part of the Community Earth System Model (CESM) and the source code is available at <http://www.cesm.ucar.edu>. DART is available at <https://www.image.ucar.edu/DARes/DART/>. The Level 2 data used in this study are available at the GOLD Science Data Center (<https://gold.cs.ucf.edu/search/>) and at NASA's Space Physics Data Facility (<https://spdf.gsfc.nasa.gov/pub/data/gold/level2/tdisk/>). The assimilation and simulation data used in this work are available at <https://doi.org/10.5281/zenodo.5546491>.

References

- Aa, E., Liu, S., Huang, W., Shi, L., Gong, J., Chen, Y., ... Li, J. (2016, June). Regional 3-d ionospheric electron density specification on the basis of data assimilation of ground-based GNSS and radio occultation data. *Space Weather*, *14*(6), 433–448. doi: 10.1002/2016sw001363
- Aksnes, A., Eastes, R., Budzien, S., & Dymond, K. (2006). Neutral temperatures in the lower thermosphere from N₂ Lyman-Birge-Hopfield (LBH) band profiles. *Geophysical Research Letters*, *33*(15). doi: 10.1029/2006gl026255
- Anderson, J., Hoar, T., Raeder, K., Liu, H., Collins, N., Torn, R., & Avellano, A. (2009, September). The data assimilation research testbed: A community facility. *Bulletin of the American Meteorological Society*, *90*(9), 1283–1296. doi: 10.1175/2009bams2618.1
- Anderson, J. L. (2001, December). An ensemble adjustment kalman filter for data assimilation. *Monthly Weather Review*, *129*(12), 2884–2903. doi: 10.1175/1520

- 413 -0493(2001)129(2884:aeakff)2.0.co;2
- 414 Bust, G. S., Garner, T. W., & Gaussiran II, T. L. (2004). Ionospheric data as-
 415 simulation three-dimensional (IDA3D): A global, multisensor, electron density
 416 specification algorithm. *Journal of Geophysical Research: Space Physics*,
 417 *109*(A11). doi: 10.1029/2003ja010234
- 418 Bust, G. S., & Immel, T. J. (2020, March). IDA4D: Ionospheric data assimilation
 419 for the ICON mission. *Space Science Reviews*, *216*(3). doi: 10.1007/s11214-020
 420 -00648-z
- 421 Cantrall, C. E., Matsuo, T., & Solomon, S. C. (2019, October). Upper atmosphere
 422 radiance data assimilation: A feasibility study for GOLD far ultraviolet obser-
 423 vations. *Journal of Geophysical Research: Space Physics*, *124*(10), 8154–8164.
 424 doi: 10.1029/2019ja026910
- 425 Chen, C. H., Lin, C. H., Matsuo, T., Chen, W. H., Lee, I. T., Liu, J. Y., ... Hsu,
 426 C. T. (2016, June). Ionospheric data assimilation with thermosphere-
 427 ionosphere-electrodynamics general circulation model and GPS-TEC dur-
 428 ing geomagnetic storm conditions. *Journal of Geophysical Research: Space*
 429 *Physics*, *121*(6), 5708–5722. doi: 10.1002/2015ja021787
- 430 Codrescu, M. V., Fuller-Rowell, T. J., & Minter, C. F. (2004, November). An
 431 ensemble-type kalman filter for neutral thermospheric composition during
 432 geomagnetic storms. *Space Weather*, *2*(11). doi: 10.1029/2004sw000088
- 433 Codrescu, S. M., Codrescu, M. V., & Fedrizzi, M. (2018, January). An ensemble
 434 kalman filter for the thermosphere-ionosphere. *Space Weather*, *16*(1), 57–68.
 435 doi: 10.1002/2017sw001752
- 436 Correira, J., Lumpe, J. D., Evans, J. S., Kyrwonos, A., Veibell, V., McClintock,
 437 W. E., & Eastes, R. (2020). Thermospheric composition and solar euv flux
 438 from the global-scale observations of the limb and disk (gold) mission. *Earth*
 439 *and Space Science Open Archive*, *31*. doi: 10.1002/essoar.10501920.2
- 440 Datta-Barua, S., Bust, G. S., & Crowley, G. (2013, November). First storm-time
 441 plasma velocity estimates from high-resolution ionospheric data assimilation.
 442 *Journal of Geophysical Research: Space Physics*, *118*(11), 7458–7471. doi:
 443 10.1002/2013ja019153
- 444 Eastes, R. W., McClintock, W. E., Burns, A. G., Anderson, D. N., Andersson,
 445 L., Aryal, S., ... Woods, T. N. (2020, June). Initial observations by the

- 446 GOLD mission. *Journal of Geophysical Research: Space Physics*, 125(7). doi:
447 10.1029/2020ja027823
- 448 Eastes, R. W., Solomon, S. C., Daniell, R. E., Anderson, D. N., Burns, A. G., Eng-
449 land, S. L., ... McClintock, W. E. (2019, August). Global-scale observations
450 of the equatorial ionization anomaly. *Geophysical Research Letters*, 46(16),
451 9318–9326. doi: 10.1029/2019gl084199
- 452 Forsythe, V. V., Azeem, I., Blay, R., Crowley, G., Makarevich, R. A., & Wu,
453 W. (2021, April). Data assimilation retrieval of electron density pro-
454 files from ionosonde virtual height data. *Radio Science*, 56(5). doi:
455 10.1029/2021rs007264
- 456 Gelaro, R., McCarty, W., Suárez, M. J., Todling, R., Molod, A., Takacs, L., ...
457 Zhao, B. (2017, July). The modern-era retrospective analysis for research and
458 applications, version 2 (MERRA-2). *Journal of Climate*, 30(14), 5419–5454.
459 doi: 10.1175/jcli-d-16-0758.1
- 460 He, J., Yue, X., Le, H., Ren, Z., & Wan, W. (2020, March). Evaluation on the
461 quasi-realistic ionospheric prediction using an ensemble kalman filter data
462 assimilation algorithm. *Space Weather*, 18(3). doi: 10.1029/2019sw002410
- 463 Hersbach, H., Bell, B., Berrisford, P., Hirahara, S., Horányi, A., Muñoz-Sabater,
464 J., ... Thépaut, J.-N. (2020, June). The ERA5 global reanalysis. *Quar-
465 terly Journal of the Royal Meteorological Society*, 146(730), 1999–2049. doi:
466 10.1002/qj.3803
- 467 Kodikara, T., Zhang, K., Pedatella, N. M., & Borries, C. (2021, May). The im-
468 pact of solar activity on forecasting the upper atmosphere via assimilation of
469 electron density data. *Space Weather*, 19(5). doi: 10.1029/2020sw002660
- 470 Krywonos, A., Murray, D. J., Eastes, R. W., Aksnes, A., Budzien, S. A., & Daniell,
471 R. E. (2012, September). Remote sensing of neutral temperatures in the
472 Earth’s thermosphere using the Lyman-Birge-Hopfield bands of N₂: Compar-
473 isons with satellite drag data. *Journal of Geophysical Research: Space Physics*,
474 117(A9). doi: 10.1029/2011ja017226
- 475 Laskar, F. I., Eastes, R. W., Codrescu, M. V., Evans, J. S., Burns, A. G., Wang,
476 W., ... Cai, X. (2021, August). Response of GOLD retrieved thermospheric
477 temperatures to geomagnetic activities of varying magnitudes. *Geophysical
478 Research Letters*, 48(15). doi: 10.1029/2021gl093905

- 479 Laskar, F. I., Eastes, R. W., Martinis, C. R., Daniell, R. E., Pedatella, N. M., Burns,
480 A. G., ... Codrescu, M. V. (2020, July). Early morning equatorial ionization
481 anomaly from GOLD observations. *Journal of Geophysical Research: Space*
482 *Physics*, 125(7). doi: 10.1029/2019ja027487
- 483 Laskar, F. I., McCormack, J. P., Chau, J. L., Pallamraju, D., Hoffmann, P., &
484 Singh, R. P. (2019, August). Interhemispheric meridional circulation dur-
485 ing sudden stratospheric warming. *Journal of Geophysical Research: Space*
486 *Physics*, 124(8), 7112–7122. doi: 10.1029/2018ja026424
- 487 Laskar, F. I., Pedatella, N. M., Codrescu, M. V., Eastes, R. W., Evans, J. S., Burns,
488 A. G., & McClintock, W. (2021, January). Impact of GOLD retrieved thermo-
489 spheric temperatures on a whole atmosphere data assimilation model. *Journal*
490 *of Geophysical Research: Space Physics*, 126(1). doi: 10.1029/2020ja028646
- 491 Lee, I. T., Matsuo, T., Richmond, A. D., Liu, J. Y., Wang, W., Lin, C. H., ...
492 Chen, M. Q. (2012). Assimilation of formosat-3/cosmic electron density
493 profiles into a coupled thermosphere/ionosphere model using ensemble kalman
494 filtering. *Journal of Geophysical Research: Space Physics*, 117(A10). doi:
495 <https://doi.org/10.1029/2012JA017700>
- 496 Lin, C. Y., Matsuo, T., Liu, J. Y., Lin, C. H., Tsai, H. F., & Araujo-Pradere,
497 E. A. (2015, January). Ionospheric assimilation of radio occultation and
498 ground-based GPS data using non-stationary background model error co-
499 variance. *Atmospheric Measurement Techniques*, 8(1), 171–182. doi:
500 10.5194/amt-8-171-2015
- 501 Liu, H.-L., Bardeen, C. G., Foster, B. T., Lauritzen, P., Liu, J., Lu, G., ... Wang,
502 W. (2018, February). Development and validation of the whole atmosphere
503 community climate model with thermosphere and ionosphere extension
504 (WACCM-x 2.0). *Journal of Advances in Modeling Earth Systems*, 10(2),
505 381–402. doi: 10.1002/2017ms001232
- 506 Marsh, D. R. (2011). Chemical–dynamical coupling in the mesosphere and lower
507 thermosphere. In *Aeronomy of the earths atmosphere and ionosphere* (pp. 3–
508 17). Springer Netherlands. doi: 10.1007/978-94-007-0326-1_1
- 509 Matsuo, T., Lee, I.-T., & Anderson, J. L. (2013, March). Thermospheric mass den-
510 sity specification using an ensemble kalman filter. *Journal of Geophysical Re-*
511 *search: Space Physics*, 118(3), 1339–1350. doi: 10.1002/jgra.50162

- McClintock, W. E., Eastes, R. W., Beland, S., Bryant, K. B., Burns, A. G., Cor-
reira, J., . . . Veibel, V. (2020, May). Global-scale observations of the limb
and disk mission implementation: 2. observations, data pipeline, and level 1
data products. *Journal of Geophysical Research: Space Physics*, *125*(5). doi:
10.1029/2020ja027809
- McCormack, J. P., Harvey, V. L., Pedatella, N., Koshin, D., Sato, K., Coy, L., . . .
Holt, L. A. (2021). Intercomparison of middle atmospheric meteorological
analyses for the northern hemisphere winter 2009-2010. *Atmospheric Chem-
istry and Physics Discussions*, *2021*, 1–48. doi: 10.5194/acp-2021-224
- McCormack, J. P., Hoppel, K., Kuhl, D., de Wit, R., Stober, G., Espy, P., . . . Hi-
bbins, R. (2017, February). Comparison of mesospheric winds from a high-
altitude meteorological analysis system and meteor radar observations during
the boreal winters of 2009–2010 and 2012–2013. *Journal of Atmospheric and
Solar-Terrestrial Physics*, *154*, 132–166. doi: 10.1016/j.jastp.2016.12.007
- Mehta, P. M., Linares, R., & Sutton, E. K. (2018, May). A quasi-physical dy-
namic reduced order model for thermospheric mass density via hermitian
space-dynamic mode decomposition. *Space Weather*, *16*(5), 569–588. doi:
10.1029/2018sw001840
- Pedatella, N. M., Anderson, J. L., Chen, C. H., Raeder, K., Liu, J., Liu, H.-L., &
Lin, C. H. (2020, September). Assimilation of ionosphere observations in the
whole atmosphere community climate model with thermosphere-ionosphere
EXtension (WACCMX). *Journal of Geophysical Research: Space Physics*,
125(9). doi: 10.1029/2020ja028251
- Pedatella, N. M., Liu, H.-L., Marsh, D. R., Raeder, K., Anderson, J. L., Chau, J. L.,
. . . Siddiqui, T. A. (2018, April). Analysis and hindcast experiments of the
2009 sudden stratospheric warming in WACCMX+DART. *Journal of Geophys-
ical Research: Space Physics*, *123*(4), 3131–3153. doi: 10.1002/2017ja025107
- Pedatella, N. M., Raeder, K., Anderson, J. L., & Liu, H.-L. (2014, August). Ensem-
ble data assimilation in the whole atmosphere community climate model. *Jour-
nal of Geophysical Research: Atmospheres*, *119*(16), 9793–9809. doi: 10.1002/
2014jd021776
- Remsberg, E. E., Marshall, B. T., Garcia-Comas, M., Krueger, D., Lingenfelter,
G. S., Martin-Torres, J., . . . Thompson, R. E. (2008, September). Assessment

- of the quality of the version 1.07 temperature-versus-pressure profiles of the
middle atmosphere from TIMED/SABER. *Journal of Geophysical Research*,
113(D17). doi: 10.1029/2008jd010013
- Ren, D., & Lei, J. (2020, August). Evaluation of physics-based data assimilation
system driven by neutral density data from a single satellite. *Space Weather*,
18(8). doi: 10.1029/2020sw002504
- Rideout, W., & Coster, A. (2006, May). Automated GPS processing for global total
electron content data. *GPS Solutions*, 10(3), 219–228. doi: 10.1007/s10291-006
-0029-5
- Rienecker, M. M., Suarez, M. J., Gelaro, R., Todling, R., Bacmeister, J., Liu, E., ...
Woollen, J. (2011, July). MERRA: NASA’s modern-era retrospective analysis
for research and applications. *Journal of Climate*, 24(14), 3624–3648. doi:
10.1175/jcli-d-11-00015.1
- Schwartz, M. J., Lambert, A., Manney, G. L., Read, W. G., Livesey, N. J., Froide-
vaux, L., ... Wu, D. L. (2008, May). Validation of the aura microwave limb
sounder temperature and geopotential height measurements. *Journal of Geo-
physical Research*, 113(D15). doi: 10.1029/2007jd008783
- Song, R., Hattori, K., Zhang, X., & Yoshino, C. (2021, August). The three-
dimensional ionospheric electron density imaging in japan using the approx-
imate kalman filter algorithm. *Journal of Atmospheric and Solar-Terrestrial
Physics*, 219, 105628. doi: 10.1016/j.jastp.2021.105628
- Sutton, E. K. (2018, June). A new method of physics-based data assimilation for
the quiet and disturbed thermosphere. *Space Weather*, 16(6), 736–753. doi: 10
.1002/2017sw001785
- Vierinen, J., Coster, A. J., Rideout, W. C., Erickson, P. J., & Norberg, J. (2016,
March). Statistical framework for estimating GNSS bias. *Atmospheric Mea-
surement Techniques*, 9(3), 1303–1312. doi: 10.5194/amt-9-1303-2016
- Wang, H., Fuller-Rowell, T. J., Akmaev, R. A., Hu, M., Kleist, D. T., & Iredell,
M. D. (2011, December). First simulations with a whole atmosphere data
assimilation and forecast system: The january 2009 major sudden stratospheric
warming. *Journal of Geophysical Research: Space Physics*, 116(A12). doi:
10.1029/2011ja017081