Impact of GOLD Retrieved Thermospheric Temperatures on a Whole Atmosphere Data Assimilation Model

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Abstract The present investigation evaluates the assimilation of synthetic data which has properties similar to actual Global-scale Observations of the Limb and Disk (GOLD) level-2 (L2) temperatures and other conventional lower atmospheric observations. The lower atmospheric and GOLD L2 temperature ($T_{\text{L2}}$) assimilated in the Whole Atmosphere Community Climate Model with thermosphere-ionosphere eXtension using Data Assimilation Research Testbed. It is found that inclusion of the GOLD $T_{\text{L2}}$ improves the forecast root mean square error (RMSE) and bias by 5% and 71%. When compared to lower atmosphere only assimilation, the improvements in RMSE and bias are 20% and 94%. An investigation of the global diurnal westward-propagating wavenumber 1 (DW1) and local diurnal tidal characteristics shows that inclusion of the GOLD temperatures improves the DW1 by about 8% and diurnal tide by more than 17%. Larger percentage improvements in the tides are seen in the lower thermosphere. Considerable improvements in the model state are also seen at times and locations where there are no GOLD observations available. These results and the background data assimilation procedure are presented here, which demonstrate that GOLD thermospheric temperature is an excellent data set that can be used for thermospheric assimilation studies and operational purposes.

Plain Language Summary A perfect numerical model simulation of the Earth is the one that can reproduce the whole atmosphere-ionosphere-thermosphere (AIT) system at any point of time. With time, the numerical models are evolving and the simulation capabilities are enhanced with new understanding of the AIT system dynamics, but they are still far from perfect. On the other hand, if one can measure any parameter or state of the AIT system at any point of time then the numerical models will be of no use. In the absence of both the above highly ambitious extreme possibilities, both the state-of-the-art model capabilities and AIT measurements can be combined in a data assimilation framework to study the dynamics and to better understand the AIT system. The present investigation evaluates GOLD mission level-2 disk temperatures and finds that they can significantly improve the thermospheric assimilation capability.

1. Introduction

The upper atmosphere, above about 100 km, of the Earth is influenced by wave forcing from the lower atmosphere and by external solar and geomagnetic forcings. For a better understanding of the whole atmosphere-ionosphere-thermosphere (AIT) system, it is necessary to study and characterize the local and global variations. Ground-based data sets have good local time coverage but they lack global coverage. While low-earth orbiting satellite based measurements may have good global coverage, they lack local time coverage. However, imaging measurements from a geo-stationary orbit can cover a great spatial and temporal window over a part of the globe. The recently launched Global-scale Observations of the Limb and Disk (GOLD) mission images the Earth’s thermosphere with unprecedented spatial and temporal coverage (Eastes et al., 2020; Laskar et al., 2020; McClintock et al., 2020). GOLD scans the Earth’s disk from geostationary orbit for about 18.5 h a day, from 0610 UT to 0040 UT. The daylight measurements of the nitrogen ($N_2$) Lyman-Birge-Hopfield (LBH) bands in the far-ultra-violet (FUV) can be used to retrieve thermospheric temperature over about, at times, one-fourth of the globe (Eastes et al., 2020).
Despite increasing numbers of experimental measurements, the current observing system remains insufficient to fully observe many of the spatial and temporal scales that are of interest scientifically and operationally. Also, with better understanding of various atmospheric and external forcing parameters, the numerical model simulations of the whole atmosphere are improving, but they are still far from being able to capture all the AIT system dynamics. In such a scenario, both the experimental measurements and the state-of-the-art whole atmosphere models can be combined in a data assimilation framework to obtain states that are more realistic than the numerical model simulations alone. With the availability of thermospheric data set from the GOLD measurements and other local plus global observations at different altitudes of the atmosphere, an investigation of the AIT system is warranted by assimilating all these measurements.

The primary measurements from GOLD mission are FUV emissions, which can be used in data assimilation models (Cantrall et al., 2019). But in the present investigation, the thermospheric temperatures that are retrieved from the N₂ LBH bands are assimilated. This is because the temperatures retrieved from GOLD LBH band emissions are validated regularly and such retrievals have a long history (Aksnes et al., 2006; Krywonos et al., 2012; Meier et al., 2015). Moreover, investigations from a forward modeling study, using Global Airglow (GLOW) code with atmospheric parameters provided by Thermosphere-Ionosphere-Electrodynamics General Circulation Model (TIE-GCM), showed that the GLOW model underestimates the radianc compared to GOLD observations (Greer et al., 2020). Also, temperature is one of the basic state variables in most general circulation models. Thus, we assimilated the retrieved temperatures rather than the emission intensity measurements.

The thermosphere-ionosphere (TI) system can change very rapidly with the change of external forcings (e.g., Fuller-Rowell et al., 1994). Also, the lower atmospheric wave forcings influence the TI system significantly (e.g., Laskar et al., 2013). So, a whole AIT data assimilation would be of great use for investigation of the TI system (Jackson et al., 2019). Most of the earlier assimilation systems assimilated the lower atmosphere (below ~100 km) data (McCormack et al., 2017; Pedatella et al., 2014) or used TI models having a lower boundary between 80 and 100 km altitudes (Cantrall et al., 2019; Chartier et al., 2016; Chen et al., 2017; M. V. Codrescu et al., 2004; S. M. Codrescu et al., 2018; He et al., 2019; Lee et al., 2012; Rajesh et al., 2017; Sutton, 2018).

Whole atmosphere assimilation capabilities are being developed gradually and they are being extended from troposphere to TI. Most of the earlier whole atmosphere assimilation efforts were primarily restricted to assimilation of lower atmosphere observations. This is because for a proper understanding of the forcing to the upper atmosphere from below, the lower atmosphere assimilation and dynamics needs to be evaluated first. Assimilation experiments using whole atmosphere models have been performed earlier (Pedatella et al., 2018; Wang et al., 2011), but they assimilated only the lower and middle atmosphere observations from altitudes below about 100 km. Recently, whole atmosphere assimilation experiments showed a positive impact of ionosphere observations on short-term forecasts and analyses (Pedatella et al., 2020). The present investigation aims to evaluate the impact of the recently available GOLD mission thermospheric disk temperatures on a whole AIT data assimilation model when both the lower atmosphere and thermospheric observations are assimilated.

2. Model, Data, and Methodology

The main objective of this study is to assimilate and assess the impact of the GOLD disk temperature ($T_{disk}$) observations in a whole atmosphere model, for that we have used the Whole Atmosphere Community Climate Model with thermosphere-ionosphere eXtension (WACCMX). Data assimilation is implemented using the Data Assimilation Research Testbed (DART) ensemble Kalman filter. Details about the model and observations are given below.

2.1. WACCMX + DART

The recently developed 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 are similar to those in the NCAR 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 $\sim 50$ km.

To reproduce specific events in WACCMX, it is necessary to constrain the model meteorology (i.e., dynamics). The data assimilation capability in WACCMX was initially implemented by Pedatella et al. (2018) using DART (Anderson et al., 2009), which uses the ensemble Kalman filter. But the earlier adoption was limited to assimilation of observations at altitudes below 100 km. In the present investigation, the WACCMX + DART assimilation capability has been extended to thermosphere altitudes for the assimilation of GOLD L2 $T_{\text{disk}}$. As the thermospheric dynamics can change fast in response to changes in forcing conditions, we use 1 h assimilation frequency.

An essential part of ensemble data assimilation is that the ensemble members should have sufficient spread. To increase the spread in the ensemble members, we use variable external forcing parameters with standard deviations of 15 sfu and 1 in F10.7 solar flux and $Kp$ index over the ensemble members. To assess the impact of assimilating GOLD $T_{\text{disk}}$ data, we run two Observing System Simulation Experiments (OSSEs); one with synthetic observations for altitudes below about 100 km, we call it lower atmosphere only assimilation (LA) and second one is with synthetic observations from lower atmosphere plus GOLD L2 $T_{\text{disk}}$ (LA+GOLD) observations. In the LA+GOLD experiment, the LA data are assimilated at all times, though the GOLD data are only assimilated when they are available, which is between $\sim 6$ and $\sim 23$ UT. These synthetic observations are generated based on a true or reference state from a free run of WACCMX. A random error is applied to the synthetic observations based on the errors in the actual observations. All the experiments in this investigation are OSSEs (with synthetic data) and the assimilating frequency is 1 h. Ideally, we would want to use a different model to generate the synthetic observations. However, this would require generating the full set of synthetic observations from another whole atmosphere model, something that we do not easily have the capabilities to do. The study is thus partly limited due to using the same model to generate the true state and perform the assimilation experiments.

For the present OSSEs, the lower atmosphere observations include conventional meteorological observations (i.e., aircraft temperatures, radiosonde temperatures, and winds), Global Positioning System radio occultation refractivity, and temperature observations from Thermosphere Ionosphere Mesosphere Energetics Dynamics satellite Soundings of the Atmosphere using Broadband Emission Radiometer instrument and Aura Microwave Limb Sounder. The solar and geomagnetic forcing parameters for the true state are $F10.7 = 76$ sfu and $Kp = 0$. While for the OSSEs, the F10.7 has an ensemble mean value of 100 sfu and a spread of 15 sfu, resetting any F10.7 value less than 60 sfu to 60 sfu. Similarly, $Kp$ index values have a mean of 0.33 with a spread of 1, but the minimum $Kp$ value was restricted to 0. With these forcing parameters, the spread in the ensembles was sufficient for the assimilation. Based on recommendations from previous studies (e.g., Pedatella et al., 2014, 2018) and to reduce the computational load, we employ 40 member ensembles for both the OSSEs.

### 2.2. GOLD Disk Temperature ($T_{\text{disk}}$)

GOLD scans the Earth’s full disk from 0610 to 2305 UT. The $N_2$ LBH band emissions from the day-side are used to retrieve the neutral atmosphere temperatures on the disk. Temperatures are retrieved for day-side latitudes and longitudes between 70°N–70°S and 30°E–127°W. The retrieval algorithm is an extension of those previously used to derive temperature from limb measurements of LBH band intensity from the High-resolution Ionospheric and Thermospheric Spectrograph instrument (Aksnes et al., 2006; Krywonos et al., 2012). Effective neutral temperatures near 160 km altitude are retrieved by fitting the observed rotational structure of the $N_2$ LBH bands using an optimal estimation routine.

The retrieved level-2 temperatures are publicly available from the GOLD web-page, https://gold.cs.ucf.edu/. Figure 1 shows an example image of the retrieved temperatures from GOLD daytime disk observations (Figure 1a), the associated random uncertainty (Figure 1b), and a map of solar zenith angle variation over the
A higher uncertainty in temperatures can be seen in the Northern hemisphere, which is due to lower signal-to-noise ratio (SNR) corresponding to higher solar zenith angles (SZAs) measurements. Currently, temperatures like these are retrieved from unbinned level 1C (L1C) LBH radiance data. In a future release, the L1C data will be binned at 2 × 2 pixels before retrieving the disk temperatures, which will reduce the noise by about a factor of 7 (Eastes et al., 2020). Though the temperature data are noisy, there are geophysical variations in them, which are very clear in 2 × 2 L1C-pixel binning as can be seen in Eastes et al. (2020) or when noisy data are filtered out (not shown here). So, to create a set of synthetic data for the current investigation, the uncertainties assumed are a factor of 7 better than is currently available.

### 2.3. Assimilation of GOLD \( T_{\text{disk}} \) in WACCMX + DART

The daytime \( N_2 \) LBH band emissions emanate primarily from the lower thermosphere. The 136.5 nm LBH band contribution functions for some representative solar zenith angles and for nadir viewing geometry are shown in Figure 2a. A contribution function provides the altitude versus emission rate. In other words, it determines the effective altitudes of the retrieved temperatures from GOLD \( N_2 \) LBH band emissions. Note that until about 55 degrees SZA, the contribution functions have similar shapes and the peak altitudes vary by only \( \sim 10 \) km. A plot of the 0° SZA contribution function and its mathematical function fit in log(\( p/p_0 \)) coordinate, where \( p \) and \( p_0 \) are pressures at a given level and at the surface, respectively, is shown in Figure 2b. As DART uses log(\( p/p_0 \)) as vertical coordinate, we use such a logarithmic scale in the forward operator calculations. The mathematical function used in the fit is a log normal function of the form:

\[
CF_{\text{fit}} = \left(\frac{A}{\mu}\right)e^{-\frac{(\log(\frac{x}{\mu})-\mu)^2}{2\sigma^2}}
\]

Where, \( A, \mu, \sigma \) are amplitude, mean, and standard deviation of \( x \), the actual contribution function. This function is used as the forward operator, which translates the model state to what would be observed by GOLD. In other words, the forward operator weights the model temperature profile to estimate a GOLD equivalent temperature.

GOLD is capable of observing daytime Earth’s disk temperatures centered over American longitudes, which are representative of the whole LBH emission layer as shown by the contribution functions in Figure 2. To avoid any spurious correlation at altitudes and locations far from the observation point, the observations are localized in space so that there is
no direct impact at locations outside the localization volume. A plot of the vertical covariance localization factor is shown in Figure 3. The peak of the vertical localization profile is close to the peak of the contribution function, which is about 160 km (or $10^{-5}$ hPa or $-20$ in log $(p/p_0)$ coordinate). As the thermosphere, in general, maintains an isothermal state, a change in temperature at the peak altitude is expected to have a positive correlation at all altitudes in the thermosphere. Due to this characteristic of the thermosphere the localization function is chosen to be positive in the upper thermosphere, even though the contribution function is near zero at those altitudes. The horizontal localization used is standard Gaspari-Cohn type (Anderson & Lei, 2013; Gaspari & Cohn, 1999) with a half width of 0.2 radians.

3. Results and Discussion

For the present OSSE investigation, we test the assimilation of synthetic $T_{\text{disk}}$ observations in WACCMX + DART for November 9–13, 2018, where the assimilation experiments started from October 20, 2018. Figure 4 shows an example of true (a), synthetic (c), forecast (b), and analysis (d) of GOLD disk temperatures on November 13, 2018 at 15 UT. Note that the synthetic data used in these assimilations have spatial properties similar to those shown in Figure 1a. Qualitatively, the analysis state compares very well with the true state, which indicate that the data assimilation system performs well. Further diagnosis of the OSSEs is discussed below, where a quantitative estimate of the improvement is given. Note that in the assimilation setup any direct impact of the $T_{\text{disk}}$ observations are restricted to only the temperatures in WACCMX + DART.

Further diagnosis of the assimilation is performed by calculating root mean square error (RMSE) and bias between model (forecast and analysis) and synthetic $T_{\text{disk}}$ observations. Figure 5 shows the variation of
The gaps in RMSE and bias are due to lack of $T_{\text{disk}}$ observations in the nighttime. Significant improvement in RMSE and bias is observed after assimilating GOLD observations. For the LA+GOLD experiment, RMSE and bias of the analysis state improve by 5% and 71%, compared to LA+GOLD forecast state. When compared to LA only assimilation, the improvement in RMSE and bias are about 20% and 94%. GOLD, Global-scale Observations of the Limb and Disk; LA, lower atmosphere only assimilation; RMSE, root mean square error.

Figure 5 shows a comparison of the whole atmosphere temperature profiles from true state, LA only assimilation, and LA+GOLD assimilation for 14 UT (left column) and 18 UT (right column) at different locations inside GOLD’s field of view. Though there are differences between the true state and the analysis state in the LA+GOLD experiment, they are smaller compared to the LA only experiment. Note that the average solar forcing for the assimilation experiments is about 25 sfu higher than the true state solar forcing. Significant improvements are also observed (not shown here) at all hours, from 7 to 23 UT, where data are available from the GOLD disk observations. The zonal mean (ZM) temperature profiles (lower panels in Figure 6) also show significant improvement compared to the LA only assimilation. These improvements in the analysis state suggests that GOLD $T_{\text{disk}}$ improves the model state significantly.

The results in Figures 6a and 6b were for sample times and locations within the GOLD’s observing temporal and spatial windows. Whereas, in Figure 7, we show a similar comparison as that in Figure 6 but at locations outside GOLD’s field of view, to see its impact. Figures 7a and 7b show comparisons at 2 UT and 15 UT and over (65°N, 60°W) where there are no or very little observations from GOLD. Even then there is...
improvement in the LA+GOLD analysis state compared to LA analysis. While in Figures 7c and 7d, the 2 UT and 15 UT show a location on the other side of the globe at (0°S, 120°E). While there are no observations from GOLD over those locations, there are improvements compared to the LA analysis. This improvement

Figure 6. Comparison of the whole atmosphere temperature profiles from true state, lower atmosphere only assimilation (LA), and lower-atmosphere plus GOLD assimilation (LA+GOLD) for 14 UT (a & c) and 18 UT (b & d) at different locations inside the GOLD field of view. The zonal mean (ZM; c & d) in LA+GOLD also shows significant improvement compared to LA only assimilation. GOLD, Global-scale Observations of the Limb and Disk.

Figure 7. Comparison of the whole atmosphere temperature profiles between true state, lower atmosphere only assimilation (LA), and lower-atmosphere plus GOLD assimilation (LA+GOLD) for 2 UT (a & c) and 15 UT (b & d) at two locations outside the GOLD's field of view. Significant improvements are observed, even at locations and times where there are no GOLD data. GOLD, Global-scale Observations of the Limb and Disk.
in the LA+ GOLD analysis outside GOLD’s field of view suggests that there are indirect improvements in the model forecast capability. Thus the assimilation of GOLD T\textsubscript{disk} data improves the model state globally, but the impact is less at locations and times outside GOLD’s window of observations.

In Figure 8, we present a global picture of the impact of T\textsubscript{disk} assimilation on model temperatures, at a fixed pressure level (7.3 × 10\textsuperscript{-7} hPa, about 194 km), over the equator, for the 5-days of OSSEs in November 2018. We show the difference between true state and the LA only assimilation (T\textsubscript{LA}−T\textsubscript{true}, in a) and true state and LA+GOLD assimilation (T\textsubscript{LA+GOLD}−T\textsubscript{true}, in b) are shown for the 5 days during November. It can be seen that the differences (in b) are near zero at locations (110\textdegree W to 20\textdegree E, through 0\textdegree), where GOLD data are available. GOLD, Global-scale Observations of the Limb and Disk; LA, lower atmosphere only assimilation.

Figure 8. Longitudinal variation of the difference between true state and the lower atmosphere only assimilation (T\textsubscript{LA}−T\textsubscript{true}, in a) and true state and LA+GOLD assimilation (T\textsubscript{LA+GOLD}−T\textsubscript{true}, in b) are shown for the 5 days during November. It can be seen that the differences (in b) are near zero at locations (110\textdegree W to 20\textdegree E, through 0\textdegree), where GOLD data are available. GOLD, Global-scale Observations of the Limb and Disk; LA, lower atmosphere only assimilation.

We have observed above that DW1 like waves in temperatures are seen in Figure 8. Here we show the comparison of DW1 amplitudes between true, LA experiment, and LA+GOLD experiment in Figure 9a. The DW1 amplitude is highest for the LA experiment and compared to it the LA+GOLD experiment DW1 has amplitudes closer to the true state. The percentage improvement in LA+GOLD experiment DW1 and percentage difference from true state are shown in Figure 9b. The percentage improvements are greater than 7% at all the altitudes above about 130 km. Greater than 10% amplitudes are also observed in percentage improvement at altitudes below 150 km, which are mainly due to the lower values of true state DW1 tide in temperature. Though there are more than 7% improvements in DW1 after assimilation of GOLD T\textsubscript{disk}, there is still about 27% (about 10°K) difference between true and GOLD assimilated DW1. This discrepancy could be attributed to GOLD observing only about one-fourth of the globe for a portion of the day. But locally over American longitudes, the improvement is better as discussed below.

To investigate the local tides over the Americas, we have done a similar analysis as that in Figure 9, but for the local diurnal tide (DT, at 0\textdegree, 50\textdegree W), which is shown in Figure 10. Here it can be seen that the LA+GOLD
experiment DT amplitude profile is much closer to true state compared to LA experiment. Also, the improvements are more than 17% compared to LA assimilation and difference between true and LA+GOLD DT is less than 10% at thermospheric levels. As the local tide estimation is affected by interaction between global and local components (Laskar et al., 2016), the discrepancies could be attributed to difference between global and local components of all the three experiments.

4. Conclusions

A set of synthetic observation from troposphere to thermosphere is used in this investigation to evaluate the impact of GOLD disk temperature measurements on the thermospheric data assimilation and dynamics. Following are the salient findings of this investigation:

1. Assimilation of GOLD disk temperatures improves the thermospheric assimilation over the GOLD field of view and also globally
2. The model forecast RMSE and bias are improved by 5% and 71%, and the improvements are 20% and 94% when compared with lower atmosphere only assimilation. Thus, the inclusion of GOLD $T_{\text{disk}}$ in the assimilation improves the short-term forecast of the thermosphere

Figure 9. Improvement of DW1 amplitude as compared to LA assimilation experiment. (a) Altitude variation of DW1 amplitudes for true (green), LA+GOLD (red), and LA (blue) are shown. (b) Percentage difference (dashed; between true and LA) and improvement (solid; with respect to LA) in DW1 amplitudes. DW1, diurnal westward-propagating wavenumber 1; GOLD, Global-scale Observations of the Limb and Disk; LA, lower atmosphere only assimilation.

Figure 10. Improvement of local diurnal tidal (DT) amplitude as compared to LA only assimilation. (a) Altitude variation of DT amplitudes for true (green), LA+GOLD (red), and LA (blue) are shown. (b) Percentage difference (dashed; between true and LA) and improvement (solid; with respect to LA) in DT amplitudes. Global-scale Observations of the Limb and Disk; LA, lower atmosphere only assimilation.
3. The global DW1 and local diurnal tide over Americas improve by about 8% and by more than 17%, respectively upon assimilation of GOLD temperatures.

4. Though GOLD observations are only during daylight hours, it improves the night time state too. These results demonstrate that GOLD level 2 disk temperatures are an excellent set of observations, which will be of use in the future investigations of atmospheric coupling, dynamics, and operational use. As GOLD $T_{\text{disk}}$ improves the thermospheric data assimilation, the current investigation shows a promise toward better forecast capability of space weather.

Data Availability Statement

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 (http://gold.cs.ucf.edu/search/) and at NASA's Space Physics Data Facility (https://spdf.gsfc.nasa.gov/pub/data/gold/).

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