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On the importance of neutral composition and temperature measurements in the 100–200 km altitude region

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Currently, thermospheric species densities and temperatures between ~100 and 200 km are not known to the accuracy needed to fully characterize how the thermosphere transitions from a well-mixed atmosphere to a diffusively separated atmosphere with zero temperature gradient. This greatly inhibits scientific discovery attainable from either models or observations in this region, especially the understanding of mechanisms that drive thermosphere and ionospheric variability from space weather to climatological time scales. The purpose of this paper is to highlight the importance and critical need for new, global, height-resolved neutral composition (O, O_2, N_2) and temperature measurements in the new ignorosphere: the 100–200 km region of the thermosphere. We conclude with observation recommendations and requirements for new comprehensive composition and temperature measurements in the 100–200 km altitude region that would lead to significant advances in thermosphere-ionosphere science, space weather, and space climate.

KEYWORDS

thermosphere, ionosphere, temperature, mass density, composition, space weather, space climate

1 Scientific motivation and challenges

The thermosphere and ionosphere (T-I) system is forced from both above and below. From above, external forcing includes (but is not limited to) extreme ultraviolet (EUV) and X-ray radiation as well as energy and momentum input *via* coupling with the solar wind and magnetosphere. From below, a wide-ranging spectrum of vertically propagating waves of lower atmospheric origin impart their energy and momentum into the T-I system (Oberheide et al., 2015; Liu, 2016; Sassi et al., 2019). Coupling between the plasma in the ionosphere and neutrals in thermosphere *via* ion drag, chemistry, and Joule heating add even more complexity to T-I system. The primary neutral parameters that define the thermospheric state are temperature, composition, mass density, and winds, which experience variations over a wide range of spatiotemporal scales (e.g., Qian and Solomon, 2012; Emmert, 2015a) due to the energy and momentum inputs outlined above. Ultimately, neutral or thermospheric variations, together with variations in the electrodynamic forcing, drive ionospheric variations and produce the space weather of the T-I system (e.g., Rishbeth, 1998; Liu et al., 2021).

The thermosphere spans roughly 90–600 km altitude, consisting primarily of N_2, O_2, O, He, and H. The thermosphere transitions between ~100 and 120 km (e.g., Offermann et al., 2007) from a well-mixed fluid (dominated by eddy diffusion) to one dominated by molecular diffusion, whereby individual species are distributed by altitude according to their molecular masses. Above ~200 km, the thermosphere is in approximate diffusive equilibrium (Meier et al., 2001), transitioning from a molecular dominated atmosphere (N_2, O_2), to an atomic dominated regime, with O diffusing upward and becoming the major thermospheric species from ~200 to 600 km. Between ~250 and 750 km (depending on the solar cycle), O accounts for most of the thermospheric mass and therefore most of the atmospheric drag experienced by satellites and debris in low-Earth orbit. Critically, the O distribution in the mesosphere and lower thermosphere (MLT, ~50–120 km), which is controlled by the relative contributions of chemistry, diffusion, and dynamics (e.g., Yamazaki and Richmond, 2013; Jones Jr, et al., 2014b; Chang et al., 2014; Gan et al., 2015), is directly connected to mass density distribution in the upper thermosphere *via* molecular diffusion (Picone et al., 2013; Jones Jr et al., 2017; Jones Jr et al., 2018; Jones Jr et al., 2021).

Adding to the complexity of the 100–200 km region is that the thermospheric temperature profile increases steeply with altitude from ~250 K at 100 km to ~1000 K at 200 km (on average). Numerous competing heating and cooling processes govern the temperature of the thermosphere, including direct absorption of solar UV radiation, thermal interaction with the ionosphere, exothermic chemical reactions, infrared radiation by several species (including CO_2 and NO), and adiabatic heating and cooling due to dynamic motions. The connection between temperature and mass density (and therefore composition) is *via* hydrostatic balance and the ideal gas law. Variations in mass density are highly sensitive to variations in underlying temperature because increased temperature acts to expand a hydrostatic column, leading to increases in the density scale height and increased mass density at a fixed altitude. For example, a 20 K overestimate of temperature over a 10 km altitude band near 100 km will produce a ~20% overestimate of atmospheric density at higher altitudes, because the erroneously high temperature produces a more expanded air column *via* hydrostatic adjustment. Thus, in order to properly interpret mass and plasma density changes measured in the upper thermosphere from previous [e.g., Challenging Minisatellite Payload (CHAMP)] and future [e.g., Global Dynamics Constellation (GDC)] satellite missions, one must understand the temperature and composition of the 100–200 km region.

Further complicating the understanding of upper T-I variations connected with variations in the 100–200 km altitude regime is that most vertically-propagating waves (solar and lunar tides, planetary waves, Kelvin waves, gravity waves) break, dissipate, and generate secondary or higher order waves at this altitude, bringing momentum and energy from the lower atmosphere into the thermosphere. As a result, accurate modeling of neutral thermospheric composition, temperature, and ionospheric plasma density are important for satellite operations and requires a deft understanding of atmospheric waves, dynamics, and thermodynamics that modulate the neutral and plasma densities at time scales from days, months, years, to decades (e.g., Qian et al., 2009, 2013; Leonard et al., 2012; Vadas et al., 2014; Emmert, 2015b; Pedatella et al., 2016; Thayer et al., 2021). Further, wave propagation and dissipation prior to geomagnetic storms can serve to precondition thermospheric composition, dynamics, and temperature, which if unaccounted for can lead to large uncertainties in modeled plasma density calculations (e.g., Pedatella and Liu, 2018).

All the above is well supported by a rich body of scientific literature and provided strong motivation for the GDC and Dynamical Neutral Atmosphere (DYNAMIC) science missions that were among the highest priority recommendations in the 2013 Decadal Survey (National Research Council, 2013). Further, both GDC and DYNAMIC were strongly advocated for in the Decadal Survey Midterm Assessment (NASEM, 2020), with the latter receiving strong community support from the 2022 CEDAR community statements on DYNAMIC (CEDAR Science Steering Committee, 2022).

2 Current state of temperature and composition measurements in the 100–200 km region

Sophisticated whole atmosphere and/or middle and upper atmospheric models constrained with realistic lower atmosphere forcing from atmospheric prediction systems or reanalyses can reproduce some of the nuances of T-I composition and temperature in the T-I system. Since the 2013 Decadal Survey, a number of advances in understanding the composition and temperature variations in the 100–200 km region have been accomplished *via* combined data-modeling efforts.

However, temperature and composition measurements in the 100–200 km region are still very sparse, which is an obstacle to the validation and interpretation of the modeling results. Figure 1 illustrates the historical and current record of major data sets as a function of altitude and year. The only current and ongoing research measurements of major thermospheric chemical constituents and/or temperature above 105 km are from the NASA Ionospheric Connection Explore (ICON) mission (Immel et al., 2017; neutral temperature measurements only, max altitude 127 km daytime, 108 km nighttime), the NASA Global-scale Observations of the Limb and Disk (GOLD) mission (Eastes et al., 2017; temperature, a vertically integrated measurement that is of limited utility; column O/N_2 and O_2 vertical profiles, but in geostationary orbit, with limited longitudinal coverage), ground-based incoherent scatter radar

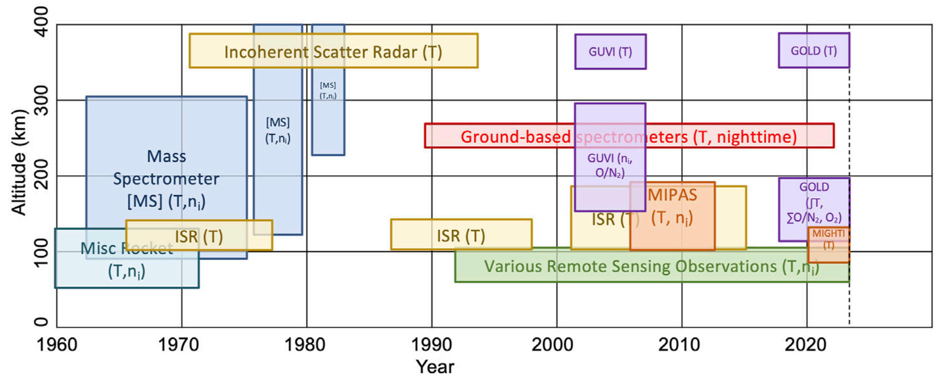

FIGURE 1
Coverage of existing and historical thermospheric composition and temperature data sets in terms of altitude and year. Note that the amount of data available within these ranges varies widely, and is generally very sparse. The dashed line indicates present day.

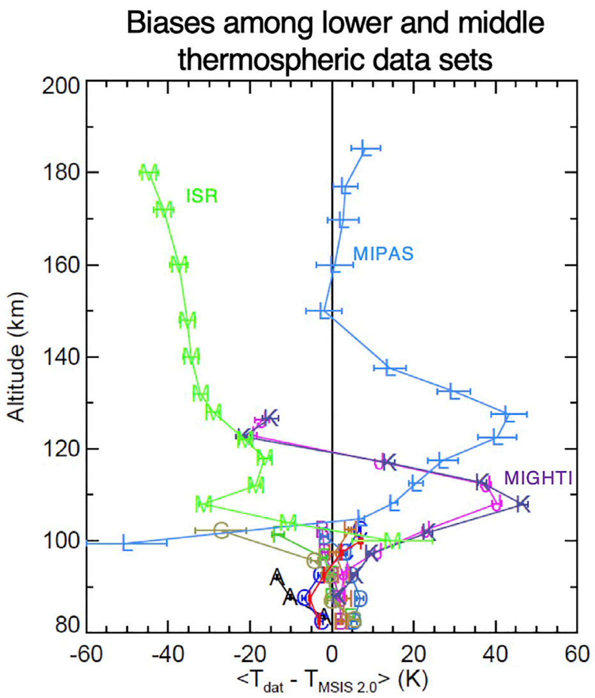

FIGURE 2
Biases among selected lower and middle thermospheric temperature datasets, during daytime and at mid-latitudes (30S—47N) with respect to NRLMSIS 2.0 as the baseline. The middle thermospheric data sets MIGHTI ("J","K"), MIPAS ("L"), and ground-based incoherent scatter radar (ISR, "M") are highlighted. The data sets below 100 km include a variety of space-based and ground-based remote sensing measurements. Error bars denote the statistical uncertainty of the estimated biases. Also shown but not discussed in are AURA/MLS ("A"), ACE/FTS ("B"), UARS/HALOE ("C"), AIM/SOFIE ("D"), Boulder, CO Lidar ("E"), Ft. Collins, CO Lidar ("F"), Logan, UT Lidar ("G"), TIMED/SABER ("H"), and ODIN/OSIRIS ("I").

(campaign-based operation, only ~3 sites, daytime only, requires special processing), ground-based airglow measurements (only at ~250 km altitude, nighttime, limited geographic coverage, sporadic temporal coverage), and ground-based resonance fluorescence lidars routinely measure temperature from ~80 km up to ~115 km at nighttime (Yuan et al., 2021), with occasional temperature observations reaching ~140 km and above (Chu et al., 2011; Liu et al., 2016). Further, important for improving the Mass Spectrometer Incoherent Scatter radar or MSIS series of empirical models with current and future thermospheric composition and temperature measurements, is the complicating factor that measurement techniques often use MSIS itself as an initial guess or for ancillary parameters needed in the retrieval (e.g., Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), Bermejo-Pantaleón et al., 2011; Global Ultraviolet Imager (GUVI), Meier et al., 2015). Thus, there is a need to expand existing and develop new techniques for measuring and retrieving thermospheric temperature and composition, especially between the 100 km and 200 km altitude region, which has strong vertical gradients and a strong influence on higher altitudes in the T-I.

In the absence of well-resolved global temperature and composition measurements the community has often turned to the empirical Mass Spectrometer Incoherent Scatter Radar (MSIS®) class of models (Hedin et al., 1977a; Hedin et al., 1977b; Hedin, 1987; Hedin, 1991; Picone et al., 2002) to understand and validate thermospheric composition and temperature phenomena in the 100–200 km region. MSIS recently went through a major reformulation and upgrade from NRLMSISE-00 to NRLMSIS version 2.0 by Emmert et al. (2021), using extensive new datasets from the ground to ~100 km altitude (green box labeled "Various Remote Sensing Observations", post-2000 in Figure 1). Further, above ~250 km new satellite drag-derived mass densities were used to tune and recalibrate thermospheric atomic oxygen.

Otherwise, the neutral parameters provided by the NRLMSISE-00 model in the thermosphere was largely retained. Emmert et al. (2021) specifically highlighted the scarcity of thermospheric composition and temperature measurements between 100 and 200 km, making the following statements, "*We also note that species densities in the middle thermosphere are not known to the accuracy needed to fully understand the critical transition from a fully mixed atmosphere to a diffusively separated one. Observations needed to constrain lower and middle thermospheric physics are scarce, and the 100–200 km region can perhaps be termed the new "ignorosphere," an epithet previously applied to the mesosphere, which by comparison is now well measured and understood.*"

Not only are thermospheric composition and temperature measurements sparse in the 100–200 km altitude region, but also existing temperature datasets exhibit large mutual biases of up to 80 K or more. For example, Figure 2 illustrates the mutual biases of selected thermospheric temperature data sets using NRLMSIS 2.0 as a benchmark, during the daytime and at mid-latitudes. Compounding the challenge of understanding the thermospheric state between 100 and 200 km and its impact on the overlying T-I system is that new "ignorosphere" overlaps the same altitude regime of the so-called "thermospheric gap", a term coined by Oberheide et al. (2011). The "thermospheric gap" refers to 110–200 km region of the thermosphere, where we know very little about the dynamics of this region due to a lack of vector wind measurements.

This lack of wind measurements coupled with the sparsity of composition and temperature measurements in the new ignorosphere has significantly hindered scientific progress on a number of T-I phenomena in which composition and temperature variations, and dynamical-control thereof, are known to play an important role. Just a few phenomena that cover both local and global spatial scales, as well as span time scales from days to beyond a solar cycle are listed below:

- Long-term trends in composition, mass density, and temperature in the thermosphere (Emmert, 2015a; Solomon et al., 2019)
- The residual interhemispheric lower thermospheric residual circulation and its effect on O and temperature (Qian and Yue, 2017).
- Characterizing the prominent drivers (especially those associated with gravity waves and tides) of the global annual and semiannual oscillations in the upper T-I, and their solar cycle variability (Jones Jr et al., 2021)
- The equinox transition of composition and temperature in the thermosphere (Qian et al., 2022).
- What actually causes changes in ∑O/N2 in existing FUV measurements, be it O, N2, or temperature and what is the contribution of each?
- Impacts of short-term (<5 days) variability of neutral constituents and temperature (e.g., Yue et al., 2016; Gan et al., 2017) between 100 and 200 km on the space weather of the upper T-I system.

TABLE 1 Key thermospheric composition and temperature observables between 100 and 200 km.

Observable	Coverage
T(z)	*Horizontal*: Global
$O(z)$, $O_2(z)$, $N_2(z)$, $H(z)$, $He(z)$	@ 500 km resolution
	Vertical: 100–300 km
	@ 5 km resolution
	Time: 24 h @ 4 but
	preferably 6 local times

3 Recommendations for addressing limitations in the "ignorosphere" and "thermospheric gap"

In the next decade, it is imperative that new and more extensive composition and temperature observations coupled with neutral wind measurements in the ignorosphere and thermospheric gap become available. Considering the scientific challenges listed above (and a number of others), Emmert et al. (2021) provided some recommendation on how to address such challenges including:

- New *in situ* mass spectrometers measurements of species densities in the thermosphere.
- New remote sensing (and potentially *in situ*) techniques for, and extensive new measurements, of height-resolved temperature and composition in the 100–200 km (and even slightly above) region.
- Dedicated research effort into identifying, characterizing, and reconciling systemic biases among existing and future composition and temperature observations.

Given these previous recommendations by Emmert et al. (2021) and others, we highly recommend flying a satellite constellation of at least 2 satellites, but ideally 3, with the necessary instruments that would provide unprecedented longitude, local time, and height-resolved temperature and composition observations of the 100–200 km region. Table 1 provides a synopsis of the new thermospheric composition and temperature observations that would facilitate new scientific discoveries in the 100–200 km region of the thermosphere. Note that these composition and temperature measurements are not much different to what was advocated for in the 2013 Decadal Survey (National Research Council, 2013) when the DYNAMIC mission was originally proposed.

Additionally, the measurements in Table 1 coupled with coincident vector wind measurements at 4 local solar times per day (2 satellites separated apart by 6 h) at the same resolution would allow one to resolve the large-scale gravity wave spectrum, daily diurnal tidal spectrum, and zonal mean wind daily. These waves are known to have profound effects on the thermospheric composition and temperature between 100 and 200 km and above (e.g., Yamazaki and Richmond, 2013; Jones Jr et al., 2014a; Vadas et al., 2014). Ideally, the composition and temperatures measurements in Table 1 coupled with coincident vector wind measurements would be measured at 6 local solar times per day (3 satellites separated apart by 4 h) at the same resolution, allowing one to resolve the daily semidiurnal tidal spectrum as well, in the altitude regime where many of these tides reach their maximum amplitude (e.g., Forbes et al., 2022). Observing the semidiurnal part of the tidal spectrum would add significant benefit as it is well-known to be important in coupling lower atmospheric variability to T-I variability in composition and temperature during sudden variability in composition and temperature during sudden stratospheric warmings (e.g., Jones Jr et al., 2020; Oberheide et al., 2020; and many others before and after these).

In closing, the lack of global, day and night, height-resolved thermospheric composition and temperature (and wind) observations between 100 and 200 km has not been sufficiently addressed since the last Decadal Survey, and continues to be an important priority for the Heliophysics community. New, comprehensive, thermospheric composition and temperature (and wind) measurements in this altitude region, would significantly advance T-I system science, space weather modeling and prediction, and provide a means for more collaboration between the ground and space-based observation communities of the 100–200 km region. A table of other Heliophysics professionals that support our position on the future of thermospheric measurements in the 100–200 km region is included as Supplementary Material.

Data availability statement

Publicly available datasets were analyzed in this study. This data can be found here: NRLMSIS 2.0 Code and all data samples used in the ensemble fits and model validation are available at https://map.nrl.navy.mil/map/pub/nrl/NRLMSIS/NRLMSIS2.0. Ground-based lidar and ISR data were obtained from http://www.cedar. openmadrigal.org website. USU Lidar data are also available online (https://doi.org/10.15142/T33H26). MIPAS data used in this study are available for registered users at http://www.imk-asf.kit.edu/english/308.php website. MIGHTI data used in this study are available at available from the ICON website (https://icon.ssl.berkeley.edu/Data) and at the Space Physics Data Facility (https://spdf.gsfc.nasa.gov/).

Author contributions

MJ and JE equally contributed to this work, and share first authorship. All authors contributed to manuscript citations, revisions, reading, and approved the submitted version.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fspas.2022.1062967/full#supplementary-material

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