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Scientific motivations and future directions of whole atmosphere modeling

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The recent development of whole atmosphere models that extend from the surface to the upper thermosphere represents a significant advance in modeling capabilities of the ionosphere-thermosphere. Whole atmosphere models have had an especially important influence on understanding the role of terrestrial weather on generating variability in the ionosphere-thermosphere. This paper provides an overview of the scientific motivations and contributions made by whole atmosphere modeling. This is followed by a discussion of future directions in whole atmosphere modeling and the science that they will enable.

KEYWORDS

whole atmosphere model, ionosphere, thermosphere, atmosphere coupling, space weather

1 Introduction

The importance of terrestrial weather on the ionosphere-thermosphere began to be widely recognized in the past few decades. Although a number of researchers had previously explored the role of the lower atmosphere on generating ionosphere-thermosphere variability [e.g., (Chen, 1992; Stening et al., 1996; Forbes et al., 2000; Rishbeth and Mendillo, 2001)], it is only more recently that this coupling is widely understood to be an important source of variability in the ionosphere-thermosphere. The considerable progress that has been made in this area can be found in a number of recent reviews (England, 2012; Pancheva and Mukhtarov, 2012; Liu, 2016; Yiğit et al., 2016; Sassi et al., 2019; Goncharenko et al., 2021; Ward et al., 2021). The increased recognition of the lower atmosphere effects on the ionosphere-thermosphere served as an important motivator for the development of whole atmosphere models, herein considered to be those that seamlessly span altitudes from the surface to the upper thermosphere (~500 km). In addition to observational investigations [e.g., (Immel et al., 2006; Chau et al., 2009; Goncharenko et al., 2010; Gasperini et al., 2020; Goncharenko et al., 2022)], the development of whole atmosphere models played a crucial role in understanding the physical mechanisms by which terrestrial weather impacts the ionosphere-thermosphere, and further confirmed the importance of the lower atmosphere on generating ionosphere-thermosphere variability.

This Perspective discusses the role of whole atmosphere models in ionosphere-thermosphere research and the future directions of whole atmosphere modeling. The focus is primarily on their role in understanding the impact of terrestrial weather on the ionosphere-thermosphere. Following a brief background on the initial development of whole atmosphere models, recent scientific progress enabled by whole atmosphere models is discussed. This is followed by a personal vision for the future of whole atmosphere model development and the science that these developments will enable.

2 Development of whole atmosphere models

A brief historical overview of the development of whole atmosphere models is first warranted in order to provide context for both recent advances and future developments. For a more detailed discussion, including what is involved in the development of a whole atmosphere model, the reader is referred to Akmaev (2011). Roble (2000) significantly advanced the concept of a whole atmosphere model by coupling together a model developed for the lower atmosphere (NCAR Community Climate Model, CCM3) with one developed for the upper atmosphere (Thermosphere-Ionosphere-Mesosphere-Electrodynamics General Circulation Model, TIME-GCM). Though viewed by Roble (2000) as a "feasibility study to determine just how processes in the lower atmosphere affect the upper atmosphere", the exploratory model proved to be highly valuable with regards to understanding coupling processes between the lower and upper atmospheres [e.g., (Liu and Roble, 2002; Mendillo et al., 2002)]. This success led to the subsequent development of several stand-alone whole atmosphere models by researchers around the world, including the Ground-to-topside model of Atmosphere and Ionosphere for Aeronomy [GAIA, (Jin et al., 2011),], HI Altitude Mechanistic general Circulation Model [HIAMCM, (Becker and Vadas, 2020)], Whole Atmosphere Model [WAM, (Akmaev et al., 2008)], and the Whole Atmosphere Community Climate Model with thermosphere-ionosphere extension [WACCM-X, (Liu et al., 2018)]. Note that in the present context, whole atmosphere models are considered those that are comprised of a single model that seamlessly extends from the surface to the upper thermosphere. Though not the focus of the present paper, it is important to recognize that a variety of other models that are not considered whole atmosphere models by this definition have also contributed significantly to the understanding of how variability in the lower atmosphere is imprinted on the middle and upper atmospheres. This includes models with upper boundaries in the lower thermosphere (~100–250 km) and models that extend into the ionosphere-thermosphere but not all the way down to the surface, as well as one- and two-dimensional models [e.g., (Hagan and Forbes, 2003; Hagan et al., 2007; Hickey et al., 2009; Qian et al., 2009; Vadas and Liu, 2009; Yiğit et al., 2009)].

One aspect of the coupled CCM3-TIMEGCM that is important to highlight is that it leveraged decades of historical model developments in what could be considered to be disparate communities. Specifically, it could not have been realized without the prior (generally separate) developments that occurred in climate and ionosphere-thermosphere modeling. Middle atmosphere models, those extending up to the mesosphere-lower thermosphere, were also of fundamental importance. Whole atmosphere models thus require expertise across a range of disciplines. Future developments will continue to require wide-ranging expertise, including atmospheric scientists, software engineers, and space physicists. While this can, at times, present a challenge, I have personally found that it makes working with whole atmosphere models full of opportunities to broaden one's perspective and learn significantly from those with a variety of areas of expertise.

3 Science enabled by whole atmosphere models

Despite their recent development, whole atmosphere models have already made significant contributions to ionosphere-thermosphere research. Some of the areas where whole atmosphere models have led to new scientific understanding are discussed below. Note that what follows is focused on the role of the lower atmosphere on generating ionosphere-thermosphere variability and it is not intended to be an exhaustive list of the scientific applications of whole atmosphere models. Other scientific topics of relevance to whole atmosphere models include long-term trends (Solomon et al., 2019; Cnossen and Maute, 2020; Liu et al., 2020) and the solar influence on chemistry and climate. All of these areas remain active areas of research and will continue to see progress with the continued development of whole atmosphere models.

The influence of SSWs on the ionosphere-thermosphere was one of the first scientific applications of stand-alone whole atmosphere models (Wang et al., 2011; Fang et al., 2012; Jin et al., 2012; Pedatella et al., 2012). Detailed discussion of the contributions of whole atmosphere models in the understanding of the coupling mechanisms between SSWs and the ionosphere-thermosphere can be found in Goncharenko et al. (2021). Notably, whole atmosphere model simulations advanced understanding of the variability of different solar and lunar tides during SSWs and their role in generating ionosphere-thermosphere variability. Another important contribution was the finding that using data assimilation systems to initialize whole atmosphere model forecasts could lead to forecasting the SSW effects on the ionosphere ~10 days in advance (Wang et al., 2014; Pedatella et al., 2018). This demonstrates the potential increased space weather forecast skill that may be obtained by incorporating lower atmospheric effects, especially during periods of strong lower atmospheric forcing.

Observational studies have long shown that the lower atmosphere contributes a significant fraction of the day-to-day ionosphere variability. The advent of whole atmosphere models has helped to quantify the variability in the ionosphere-thermosphere that is driven by the lower atmosphere. Model simulations by Fang et al. (2018) have shown that the lower atmosphere contributes ~10–20% of the ionosphere variability. This is generally consistent with prior observational estimates, demonstrating that whole atmosphere models can reasonably represent the day-to-day variability of the ionosphere. Additional modeling studies have shown that there exists large day-to-day variability in atmospheric tides and planetary waves and that these are likely to be the source of the persistent day-to-day variability in the ionosphere [e.g., (Jin et al., 2011; McDonald et al., 2018; Gasperini et al., 2020; Liu, 2020)].

Though whole atmosphere models are typically run at a relatively coarse resolution (1-2°), the development of models with resolutions of 0.25–0.50° has enabled investigation into smaller scale variability. High resolution whole atmosphere model simulations have led to new understanding of the pathways by which gravity waves reach the thermosphere where they can imprint themselves on the ionosphere by generating traveling ionospheric disturbances (TIDs) at middle latitudes and plasma instabilities in the equatorial region. Though previous research investigated the impacts of gravity waves on the thermosphere [e.g., (Vadas and Fritts, 2004; Vadas and Liu, 2009; Yiğit et al., 2009; Yiğit and Medvedev, 2009)], high resolution whole atmosphere model simulations by Vadas and Becker (2019) and Becker and Vadas (2020) provided new insight into the gravity waves reaching the thermosphere, which include an important contribution from secondary and higher-order waves that are generated by the momentum deposition that results from wave breaking. Complete understanding of this process for gravity waves to reach the thermosphere would be difficult without high resolution whole atmosphere modeling owing to the difficulty in observing gravity waves throughout their full altitude range. The capability to simulate small-scale waves in the thermosphere enabled by high resolution models further enables simulations of small-scale structures in the ionosphere, such as TIDs and equatorial instabilities (Miyoshi et al., 2018; Huba and Liu, 2020).

An important feature of whole atmosphere models is that they can simultaneously capture ionosphere-thermosphere variability that is driven by the lower atmosphere as well as variability due to solar and geomagnetic activity. This is critical as solar and geomagnetically driven variability occurs on top of the background state of the ionosphere-thermosphere, which is in-part controlled by waves propagating upwards from the lower atmosphere. Previous studies (Hagan et al., 2015; Pedatella, 2016) found that incorporation of lower atmospheric effects can significantly alter the simulated response to a geomagnetic storm. This was confirmed in the context of a whole atmosphere model by Pedatella and Liu (2018), who found that regional differences in the ionosphere-thermosphere response to a geomagnetic storm can reach 50–100% due to lower atmospheric effects.

4 Future of whole atmosphere modeling

Whole atmosphere models will continue to play a critical role in enabling scientific understanding of the ionosphere-thermosphere system. It is likely that they will also have an increasing role operationally, as evidenced by the recent implementation of the NOAA WAM for operational space weather forecasting (https://www.swpc.noaa.gov/products/wam-ipe). Here I outline a number of areas for advances in model development along with how they will facilitate advances in ionosphere-thermosphere research and space weather operations.

Fully capturing the range of spatial scales that influence the ionosphere-thermosphere requires high-resolution whole atmosphere models. Initial high-resolution whole atmosphere model simulations with horizontal resolutions of ~0.25–0.50° have shown the profound influence of small-scale waves on the thermosphere-ionosphere, including the generation of equatorial ionosphere instabilities (Huba and Liu, 2020). Such high-resolution capabilities have only been developed in the past several years and have yet to be fully exploited in terms of understanding the influence of atmospheric waves of various scale sizes on the ionosphere-thermosphere. At the same time, it is also crucial to continue advancing the development of high-resolution modeling capabilities. Current models rely on hydrostatic dynamical cores, which inherently limits their ability to simulate the full extent of the waves that influence the ionosphere-thermosphere. This can be addressed by adopting non-hydrostatic dynamical cores, though incorporating a non-hydrostatic dynamical core is nontrivial owing in-part to the need to control dynamical instabilities (Griffin and Thuburn, 2018). Minimizing unphysical noise, for example through hyperdiffusion or hyperviscosity (Dennis et al., 2012; Ullrich et al., 2018), is also critical to separate real wave variability from unphysical noise. The development of new dynamical cores allows for regionally refined grids, enabling extremely high resolutions [O (5–10 km)] over specific areas within a coarser resolution global grid. Regionally refined grids have yet to be employed in whole atmosphere models, though they are likely the only feasible approach to obtain resolutions on the order of 5–10 km within the context of a global model in the foreseeable future. Important scientific questions that can be addressed through the continued development and application of high-resolution whole atmosphere models include cross-scale wave coupling processes and the mechanisms responsible for the day-to-day variability of small-scale ionospheric structures, such as TIDs and equatorial irregularities.

High-resolution simulations will continue to be inhibited by their computational demands, restricting their applications to simulation lengths on the order of years. There will thus continue to be a need for whole atmosphere model configurations with coarser resolutions (~1-2° degrees) for certain applications (e.g., long-term trends, multi-year climatological studies, etc.). These resolutions necessitate parameterization of the atmospheric gravity waves that influence the middle and upper atmospheres. Though critical for reproducing the mean state of the middle and upper atmosphere, gravity wave parameterizations remain a significant source of uncertainty in whole atmosphere models (Pedatella et al., 2014). This is partly due to the fact that many existing gravity wave parameterizations rely on a number of assumptions, such as strictly vertical and instantaneous propagation, that are known to be incorrect. Updated gravity wave parameterization schemes may alleviate some of the uncertainty due to gravity wave parameterizations [e.g., (Yiğit et al., 2008; Bölöni et al., 2021)]. They additionally neglect secondary and higher-order waves that are now thought to have an increasingly important role at higher altitudes (Becker and Vadas, 2020). It is important to note that even high-resolution whole atmosphere models will continue to rely on parameterized processes for the near future. This is due to the fact that certain processes, such as convective generation of gravity waves, wave dissipation, and mixing, will continue to be on sub-grid scales. Development of improved parameterization schemes for both high- and low-resolution whole atmosphere models will therefore be necessary to address existing uncertainties in whole atmosphere models.

While a number of data assimilation systems have been developed that extend into the lower thermosphere [e.g., (Wang et al., 2011; Eckermann et al., 2018; Koshin et al., 2020)], a true whole atmosphere data assimilation system that assimilates observations from the surface to the ionosphere-thermosphere has only recently been realized (Pedatella et al., 2020). There thus remains considerable room for improvement in current data assimilation capabilities for whole atmosphere models. Data assimilation systems have been extensively used for numerical weather prediction (NWP), again providing the opportunity to leverage the extensive prior developments in a different discipline. However, data assimilation systems need to be tailored to the specific demands of whole atmosphere models owing to differences between the troposphere-stratosphere and ionosphere-thermosphere. Important differences that influence the data assimilation system include different spatial and temporal scales of the dynamical variability, greater influence of external driving in the ionosphere-thermosphere compared to the troposphere, less understanding of model error characteristics in the ionosphere-thermosphere, and the relative sparsity of observations compared to the troposphere. Dealing with unbalanced adjustments, which can generate spurious waves, will also be critical due to the large wave growth with altitude. The development of high-quality whole atmosphere data assimilation systems will provide the opportunity to advance a wide-range of scientific areas of interest to the space physics community, much in the way that atmospheric reanalysis products (e.g., ERA-5, MERRA2) are widely used across the atmospheric science research community. Furthermore, whole atmosphere data assimilation systems can provide initial conditions for space weather forecasting, enabling the study of the predictability and forecast skill of the ionosphere-thermosphere, an area that is vastly understudied in the authors opinion. Development of whole atmosphere data assimilation systems is also critical for operational space weather forecasting, especially for forecasting the day-to-day variability of the ionosphere-thermosphere during periods of quiet solar and geomagnetic activity.

Though slightly outside the primary focus of the present article, it should be noted that improvements to the specification of high-latitude forcing in whole atmosphere models are also required. Whole atmosphere models currently typically rely on empirical specifications of the high-latitude electric potential and auroral precipitation that are known to be deficient. Improvements in the high-latitude forcing may be realized through data-driven approaches, such as the Assimilative Mapping of Ionosphere Electrodynamics [AMIE, (Richmond and Kamide, 1988)] and Assimilative Mapping of Geospace Observations [AMGeO, (Matsuo, 2020)]. Coupling with a magnetospheric model is an alternative approach, and has proven to be beneficial for improving the high-latitude forcing specification in ionosphere-thermosphere simulations (Wang et al., 2004; Pham et al., 2022). Additionally, the current capability of whole atmosphere models to simulate the effects of particle precipitation on the chemistry of the middle atmosphere is inhibited by large uncertainties in the particle precipitation [e.g., (Nesse Tyssøy et al., 2022; Sinnhuber et al., 2022)]. Improved specifications of particle precipitation will enable better representation of solar influences on chemistry and climate.

It is important to recognize that although the above advances in whole atmosphere modeling and data assimilation capabilities will themselves enable new understanding of the ionosphere-thermosphere, it remains important to continually assess the fidelity of model simulations. This entails both confronting the model with observations as well as performing detailed inter-model comparisons. Such comparisons provide crucial insight into model shortcomings and can help identify areas for future development. Observational verification of whole atmosphere models is especially critical; however, it is inhibited by the deficiency of observations, especially in the thermosphere. A robust observing system is thus essential for ensuring the continued advancement of whole atmosphere models.

5 Conclusion

The development of whole atmosphere models have significantly advanced our understanding of the influence of the lower atmosphere on the ionosphere-thermosphere across a range of temporal and spatial scales. The advances outlined above will serve to advance our existing modeling capabilities, leading to new understanding of the processes that generate ionosphere-thermosphere variability. Some of the important scientific topics that can be addressed with advanced whole atmosphere modeling capabilities include: 1) the influence of terrestrial weather on the day-to-day variability of the ionosphere, including TIDs and equatorial irregularities; 2) cross-scale coupling between small and large scale waves; 3) long-term trends; 4) predictability of the ionosphere-thermosphere; 5) interaction between lower atmosphere and solar/geomagnetic driven variability; and 6) solar influences on atmospheric chemistry and climate. Advances in whole atmosphere modeling will thus enable new understanding across a range scientific areas, demonstrating the need to continue advancing current modeling capabilities. They may additionally serve to improve operational space weather forecasts.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

Author contributions

The author confirms being the sole contributor of this work and has approved it for publication.

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Conflict of interest

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

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Publisher's note

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