Future Directions for Whole Atmosphere Modelling: Developments in the context of space weather

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Key Points:

- We have reached a paradigm shift, where any self-respecting space weather model of the upper atmosphere now needs to have some representation of the lower atmosphere.
- Further model developments are required in several key areas, including dynamical cores and the improved representation of gravity waves.
- A roadmap of future actions is presented to ensure good progress continues to be made. This includes the development of a multi-model verification strategy.

Abstract

Coupled Sun-to-Earth models represent a key part of the future development of space weather forecasting. With respect to predicting the state of the thermosphere and ionosphere, there has been a recent paradigm shift; it is now clear that any self-respecting model of this region needs to include some representation of forcing from the lower atmosphere, as well as solar and geomagnetic forcing. Here we assess existing modeling capability and set out a roadmap for the important next steps needed to ensure further advances. These steps include a model verification strategy, analysis of the impact of non-hydrostatic dynamical cores, and a cost-benefit analysis of model chemistry for weather and climate applications.

Plain Language Summary

Numerical models that comprehensively simulate the region between the Sun and the Earth represent a key part of the future development of space weather forecasting. With respect to predicting the Earth's upper atmosphere, there has been a recent paradigm shift; it is now clear that any self-respecting model of this region needs to include some representation of impacts from below (the lower atmosphere) as well as from above (solar variability and the effects of solar wind fluctuations). Here we assess existing modeling capability and set out a roadmap for the important next steps needed to ensure further advances. These steps include a strategy for checking the accuracy of the models, an analysis of the impact of methods chosen to represent upper atmosphere dynamics, and an assessment of the relative benefits of comprehensive (but expensive) and simplified (but inexpensive) model representations of upper atmosphere chemistry.

1. Introduction

We are at the stage in the development of operational space weather forecasts where individual models of components of the Sun-to-Earth domain (including the ionosphere and the thermosphere) are beginning to be coupled together. Such a coupled modelling system, constrained by assimilation of near real time observations, has the potential to provide considerably better forecasts than currently available. It is clear that representing the impact of, for example, a Coronal Mass Ejection, across the whole Sun-to-Earth domain can potentially improve forecasts in the ionosphere. The potential for improved forecasts has already been demonstrated for parts of the Sun to Earth system. For example, coupling a global magnetosphere model with an inner magnetosphere drift physics model considerably improves forecasts of geomagnetic storms (Liemohn et al., 2018), and improved representation of the thermosphere leads to improved ionospheric evolution (e.g. Chartier et al., 2013). In addition, there is a strong connection between the lower atmosphere state and the ionosphere that was highlighted initially by Immel et al. (2006) and demonstrated in later modelling studies (eg Pedatella et al., 2016). Furthermore, data assimilation schemes are already used for operational ionosphere models (e.g. Schunk et al., 2016) and experimental systems show that assimilation can improve model initial conditions in the thermosphere (e.g. Murray et al.,2015), the magnetosphere (e.g. Merkin et al., 2016) and the heliosphere (e.g. Lang et al., 2019).

However, it is also becoming increasingly apparent that, in addition to correctly specifying this space weather forcing, thermosphere and ionosphere forecasts can also benefit from an accurate representation of coupling from within and below. The motivation for a whole atmosphere model (i.e., a model that extends from the ground up to the exobase) is thus two-fold:

- Recent research (e.g., Chartier et al., 2013, 2016, Hsu et al., 2014) has shown that, no matter how accurately one represents the current ionospheric state, the quality of the subsequent ionospheric forecasts crucially depends on the ability to also represent the thermosphere and its evolution.
- Both the ionosphere and thermosphere are sensitive to forcing from the lower atmosphere. The seminal paper by Immel et al. (2006) indicated connections between tidal patterns in the lower thermosphere and the F-region ionosphere, and noted that the tidal structure was linked to patterns of convection in the equatorial troposphere. Furthermore, numerous papers (e.g. Liu and Roble, 2002, Goncharenko et al., 2010a, 2010b, McDonald et al., 2018, Pedatella et al., 2012) have shown how planetary wave forcing, specifically via stratospheric sudden warmings (SSWs), can affect lower thermospheric tides and thus the ionosphere.

Akmaev (2011) reviewed whole atmosphere models at a time when these models were quite new and our understanding of the links between the lower and upper atmosphere was developing. A Whole Atmosphere Modelling Workshop was held in Tres Cantos, Spain in June 2018 and a strong consensus emerged: the need to have some representation of the lower atmosphere in space weather models of the upper atmosphere. This is highly significant for the continued development of whole atmosphere models. In this commentary we review existing models, how their building blocks can be further developed, and how we can use observations (via data assimilation and verification) to confront the model simulations and potentially produce improved forecasts.

2. Existing Models

There are three current whole atmosphere space weather models:

- The Whole Atmosphere Model (WAM) (Akmaev et al., 2008, Fuller-Rowell et al., 2008) is based on the US National Weather Service Numerical Weather prediction model and extends from the surface to around 600 km. It is being combined with a separate ionosphere model Ionosphere Plasmasphere Electrodynamics (IPE; Maruyama et al., 2015) to produce a coupled model of the ionosphere and neutral atmosphere. WAM represents both the mean state and tides in the thermosphere well (e.g Lieberman et al., 2013 show good agreement with diurnal and time mean Challenging Mini Satellite Payload (CHAMP) winds). The pattern of changes seen in ionospheric vertical plasma drift and Total Electron Content (TEC) (that occur in response to SSW forcing from below) agrees well with observations (e.g. Wang et al., 2014).

- The Whole Atmosphere Community Climate Model with thermosphere and ionosphere extension (WACCM-X (Liu et al., 2010, Liu et al., 2018) is focused primarily on **climate** timescales (in contrast to WAM, which is focused on **weather** forecast timescales). With a comparable altitude range to WAM, it has a much more detailed representation of neutral and ion chemistry. Liu et al (2018) report that in WACCM-X the amplitudes and seasonal variations of atmospheric tides in the mesosphere and lower thermosphere (MLT), equatorial ionosphere anomaly structures and storm-time ionospheric behavior are all in good agreement with observations.

- The Ground to topside model of the Atmosphere and Ionosphere for Aeronomy (GAIA) combines neutral atmosphere, ionospheric and electrodynamic models. The neutral model covers the entire atmosphere from the Earth's surface up to the top of the thermosphere and contains a comprehensive range of physical parametrizations (e.g. Fujiwara and Miyoshi, 2010). Jin et al. (2012) show the ability of GAIA to model the impact of an SSW on migrating tides and the associated ionospheric response, with in general good agreement shown with Sounding of the Atmosphere using Broadband Emission (SABER) and Constellation Observing System for Meteorology, Ionosphere, and Climate (COSMIC) observations.

[For clarification: **weather** models focus on short forecast timescales (often less than 10 days), and use as fine a resolution as possible in order to represent meteorological features such as weather fronts. Since forecast quality will depend on initial conditions, weather models must be initialized using data assimilation. Coupling to other models (such as an ocean model) is usually not required on forecast timescales, and the need to run quickly in near real time precludes the use of such coupled models and it is necessary to use fast, less complex representations of physics and chemistry. **Climate** models are run for long forecast timescales such as annual or multi-decadal periods, and so generally have coarser resolutions than weather models. Coupling to comprehensive models of the Earth system (chiefly ocean and atmospheric chemistry models) is required to represent long term variability and climate change. For the specific case of whole atmosphere models, WAM and WACCM do not completely meet the description given above (for example, WACCM can run at a finer horizontal resolution than WAM), but the WAM chemistry scheme is simple and designed for fast weather forecasts, whereas the WACCM chemistry scheme is considerably more complex, and it can be coupled to an ocean model. This enables WACCM to be used in activities like the Coupled Model Intercomparison Project 5 (CMIP5), studying, for example, climate change from 1850 (Marsh et al., 2013) and climate impacts associated with long term ozone change (Eyring et al., 2013).]

3 Building Blocks for better models

3.1 Dynamics – gravity waves and dynamical formulation

The representation of gravity waves is very important for accurate modelling of the thermosphere. They are the prime driver of the middle atmosphere circulation and affect tidal amplitudes, and thus can influence the mechanisms connecting the lower atmosphere with the thermosphere and ionosphere (see e.g. Yiğit et al., 2016). Furthermore, accurate simulation of medium and small-scale travelling ionospheric disturbances (MSTIDs), and associated ionospheric plasma bubbles which impact precision application of Global Navigation Satellite

System (GNSS) data, require the ability to represent sub grid-scale gravity waves in whole atmosphere models. This information on MSTIDs could be input into existing tools for estimating GNSS positioning error from TIDs (e.g. Lejeune et al., 2012). Gravity waves also play an important role in the transport of chemical constituents, which is discussed in more detail later.

Liu et al. (2014) ran a fine resolution (0.25^o x 0.25^o horizontal, 0.1 scale height vertical) version of WACCM to demonstrate the simulation and impact of gravity waves up to around 100 km. However, it is not clear whether such resolutions are needed at higher levels in the thermosphere. Miyoshi et al. (2018) showed that a GAIA simulation with a resolution of 1^o x 1^o produces fluctuations in electron density with length scales less than around 1000 km and periods of less than around 2 hours, which are in good agreement with observations and which are not seen in a coarser resolution (2.5^o x 2.5^o) simulation. The fluctuations reported by Miyoshi et al. are attributed to TIDs that are excited by secondary gravity waves. These waves typically have horizontal wavelengths of around 100 km to several 1000s of km (Vadas and Crowley, 2010). This also appears consistent with Gardner and Schunk (2011), who indicated observed gravity waves in the thermosphere typically have horizontal scales of around 100-500 km. Furthermore, at altitudes above around 110 km molecular viscosity and thermal conduction strongly influence gravity wave filtering and dissipation, as opposed to winds and wave breaking lower in the atmosphere (see e.g. Vadas and Fritts, 2005). Accordingly, lower atmosphere gravity wave parametrization schemes may not be appropriate in the thermosphere. Schemes that specifically focus on parameterizing gravity waves in the thermosphere (e.g.Yiğit et al., 2008) could be adopted for coarse horizontal resolution whole atmosphere model simulations.

Presently, WAM, WACCM-X and GAIA use hydrostatic dynamical cores. The dynamical core solves the governing fluid and thermodynamic equations in the model on resolved scales, while parametrizations represent sub-grid-scale processes and other processes not included in the dynamical core such as radiative transfer (Thuburn, 2008). Certainly for some applications, such as satellite drag, the hydrostatic approximation appears adequate (see e.g Bruinsma et al., 2018), but there is still a need to identify the impact on model results that may arise from non-hydrostatic processes. For some applications that require accurate representation of the wave fluctuations (such as radio wave propagation in the bottom-side F region for HF applications), the hydrostatic approximation may be inappropriate in the thermosphere, and adoption of non-hydrostatic (non-H) dynamical cores appears to be a logical next step. The hydrostatic approximation breaks in the presence of large vertical accelerations (e.g Curry and Webster, 1998), and using a non-H dynamical core may affect the modelled gravity wave spectrum, particularly when applied at fine horizontal resolution. High frequency waves with horizontal wavelength less than $4\pi H$ (where H is scale height) should be treated non-hydrostatically (Akmaev, 2011). For example, Eckermann et al. (2016) showed observations of gravity waves that had propagated from the surface to the lower thermosphere with vertical velocities of several tens of ms^{-1}. They concluded that these waves must be non-hydrostatic, since if they were hydrostatic they would have broken in the troposphere or lower stratosphere rather than propagating higher. Therefore, selection of a non-H dynamical core can affect the modelled gravity wave spectrum in the MLT, and thus the simulation of MSTIDs. A fine horizontal resolution is required to represent such waves in the first place, and, given that whole atmosphere models currently have resolutions of ~100 km to 200 km, the case for using non-H cores at such resolutions is not yet well made. Three new whole atmosphere models are being developed which use non-H cores: the Navy Global Environmental Model (NAVGEM; e.g. McCormack et al., 2017), the Met Office Extended Unified Model (UM) and WAM, where the current dynamical core is being replaced with the Geophysics Fluid Dynamics Laboratory Finite-Volume on a Cubed-Sphere (FV3) non-H core (Ullrich et al., 2017). In addition, Borchert et al. (2018) report on work to extend the ICOsahedral Non-hydrostatic (ICON) general circulation model up to 150 km altitude. NAVGEM and the UM have the option to switch between hydrostatic and non-H formulations, and both these models could play key roles in evaluating the importance of non-H cores in whole atmospheric models.

There can also be issues with the robustness of non-H dynamical cores in the thermosphere. Griffin and Thuburn (2018) showed that the UM required the addition of molecular viscosity and diffusion in order to realistically stabilize artificial wave growth, as this viscosity has a significant damping effect in the thermosphere. Another challenge arises above the turbopause (around 105 km) where diffusive separation means that air parcels are no longer turbulently mixed and the molecular weight of a species determines its dynamical evolution. Therefore, ideally each species should have its own set of dynamical equations that need to be solved. The molecular diffusion is also affected by variable gravity which in turn modifies atmospheric scale heights. Thus, there is a need to reformulate the dynamical core to properly model the individual species, as well as a need to add a correction to the thermal equation.

3.2 Radiation and chemistry

Accurate radiation and chemistry schemes are needed throughout the whole atmosphere model domain, most obviously in the MLT where the radiation scheme calculates the absorption of solar radiation that drive the large rise in temperature with height there. This means that radiation schemes need to include the far ultraviolet (FUV), extreme ultraviolet (EUV) and soft x-ray spectral ranges that are usually ignored in lower atmosphere models. In the MLT, heating from exothermic reactions becomes important (especially during polar night) and must be accounted for to correctly simulate the thermal structure. Quenching of $O(^1D)$ is a large source of heating throughout the MLT, above 100 km ion reactions and reactions involving atomic nitrogen are significant sources of heat, and below 100 km O_x and HO_x reactions are the dominant producers of chemical heating (Marsh et al., 2007). In addition, above the mid-mesosphere, local thermodynamic equilibrium (LTE) schemes need to be replaced by non-LTE formulations, since both Near Infrared heating and Infrared cooling are over-estimated by the LTE schemes. The Fomichev non-LTE parametrization (Fomichev et al., 2005, 2008; Ogibalov and Fomichev, 2003), is the only scheme currently available for Earth GCMs. Its formulation is based on recent atmospheric conditions and it lacks the adaptability to be used for climate change experiments. The UM's radiation scheme is being extended to include FUV and EUV wavelengths. The scheme is highly flexible, with the option of being run using different spectral resolutions. In future it could be further modified to include a more comprehensive representation of non-LTE heating, possibly based on a scheme developed for Mars (López-Valverde and López-Puertas, 1994), which potentially represents a considerable improvement on the Fomichev scheme. Since the scheme is also publically available it could be a highly important community resource for future collaborative whole atmosphere model development.

While only relatively few major chemical reactions are sufficient to adequately represent the large rise in temperature in the MLT (Marsh et al., 2007), other challenges remain. Below 85 km the atmospheric chemistry is dominated by compounds, and above 100 km by ion chemistry. Particularly interesting chemistry exists in between, where atoms including highly reactive hydrogen and oxygen atoms are in abundance, with maximum mixing ratios observed at around 85 km and 90-95 km, respectively (Plane et al., 2015). WACCM simulations of metal layers originating from the ablation of meteoroids in the MLT give good model agreement with data at mid latitudes, but show worse agreement at high latitudes. For example, for Fe chemistry Feng et al. (2013) shows that the model significantly overestimates winter Fe and underestimates summer Fe compared to observations from three Antarctic ground-based lidars. This implies that the model vertical transport of chemical species may be significantly underestimated. A possible issue is that global models cannot capture transport associated with small scale gravity waves, and adding diffusion terms to account for this does help with reducing the large bias. Observations of MLT chemistry are sparse, and thus there is great scope for new observations to significantly improve our knowledge of the interaction between chemistry and transport. For example, recent observations made by the Atmospheric Chemistry Experiment (ACE) indicate nitrous oxide (N_2O) is being produced in the MLT (Sheese et al., 2016). N_2O is a precursor of odd nitrogen (NO_x) which destroys stratospheric ozone. A new chemical source of N_2O has been successfully added to WACCM by Kelly et al. (2018). Model simulations were able to capture the observed N_2O layer and well replicate seasonal variations near the poles. Recent studies have also highlighted the importance of radiation and chemistry schemes working together to produce the strong NO cooling which is observed in the immediate aftermath of geomagnetic storm-time thermospheric heating (e.g. Knipp et al., 2017) .

3.3 Ionosphere and electrodynamics

The coupling between the thermosphere and ionosphere is important, as mentioned above, in ensuring a more accurate evolution of the ionospheric state. Fang et al. (2013) performed an intercomparison of a range of ionospheric models. It is clear that the thermosphere / ionosphere coupling was modelled better when the models employed a fully consistent representation of the electrodynamics. This led to the development of the IPE model, which includes the following requirements: it represents the ionosphere globally with similar resolution to the neutral atmospheric model (WAM) it is coupled to; it uses self-consistent electrodynamics for quiet and storm-time dynamo processes; it uses a coupling infrastructure.

Also important is an accurate representation of the electric field and its variation. There are limitations with current empirical electric field models, such as those developed by Heelis (1982) and Weimer (2005). These are climatological in nature, but more observations are required to capture the electric field variability. The introduction of Super Dual Auroral Radar Network (SuperDARN) data crucially adds extra observations polewards of 40^o geomagnetic latitude (as well as providing observations at lower latitudes), and the deviation of SuperDARN high latitude electric fields from the average ionospheric state shows the importance of accounting for the prior evolution of the ionospheric state. M.-T. Walach (presentation available at http://www.research.lancs.ac.uk/portal/en/activities/characterising-and-understanding-temporal-variability-in-ionospheric-flows-using-superdarn-data(21f8f287-e085-4418-8a1c-387d597ef2f0).html) used SuperDARN data to show that greater solar wind corresponds to greater variability in convection, and is currently investigating the drivers of this variability in more detail. Use of SuperDARN observations in the Canadian Ionosphere and Atmosphere Model (Martynenko et al., 2014) allows detailed features in the plasma density distribution to be reproduced, especially in the topside ionosphere at high latitudes. Data from the Assimilative Mapping of Ionospheric Electrodynamics (AMIE) can be used to assimilate multiple data sources (SuperDARN) for testing in whole atmosphere models. The electric field model chosen also influences modelled Joule heating, and it is important to continue to confront empirical model-based estimates with observations (e.g., Billett et al., 2018).

3.4 Observations for Data Assimilation and model verification

Data Assimilation (DA) is important in attempting to ensure the model state is constrained to be close to the true atmospheric state, and has been applied extensively in WACCM-X, WAM and NAVGEM. DA in WACCM-X is done using an ensemble Kalman filter while the NAVGEM DA system is a hybrid of 4D-Var and an ensemble Kalman Filter. The ensemble Kalman Filter (Evensen, 1994) is a combination of a Kalman Filter (which evolves the state and estimate covariance as new observations arrive) and Monte Carlo estimation methods (the full estimate covariance matrix is explicitly evolved using an ensemble (sample of evolved states)). The NAVGEM system has been shown to add a lot of value in the thermosphere. As an example, in Figure 1 the observed wavenumber 4 structure in TEC is best reproduced when the NAVGEM model thermosphere is forced by 3-hourly analyses; forcing by 6-hourly analyses is less accurate. A major challenge is that the models cover a large altitude range, so waves can grow exponentially, and to maintain model stability with DA, more damping is often added to deal with spurious small scale waves. A consequence of this approach is that while model dynamics and chemical transport are improved it is at the cost of the tidal amplitudes being too weak. To add to the challenge in the upper atmosphere, data are sparse and processes act on shorter time scales than in the lower atmosphere. Provision of considerably more near real time observations of the upper atmosphere, particularly of the thermosphere, is vital if we are to exploit DA in order to produce improved model forecasts.

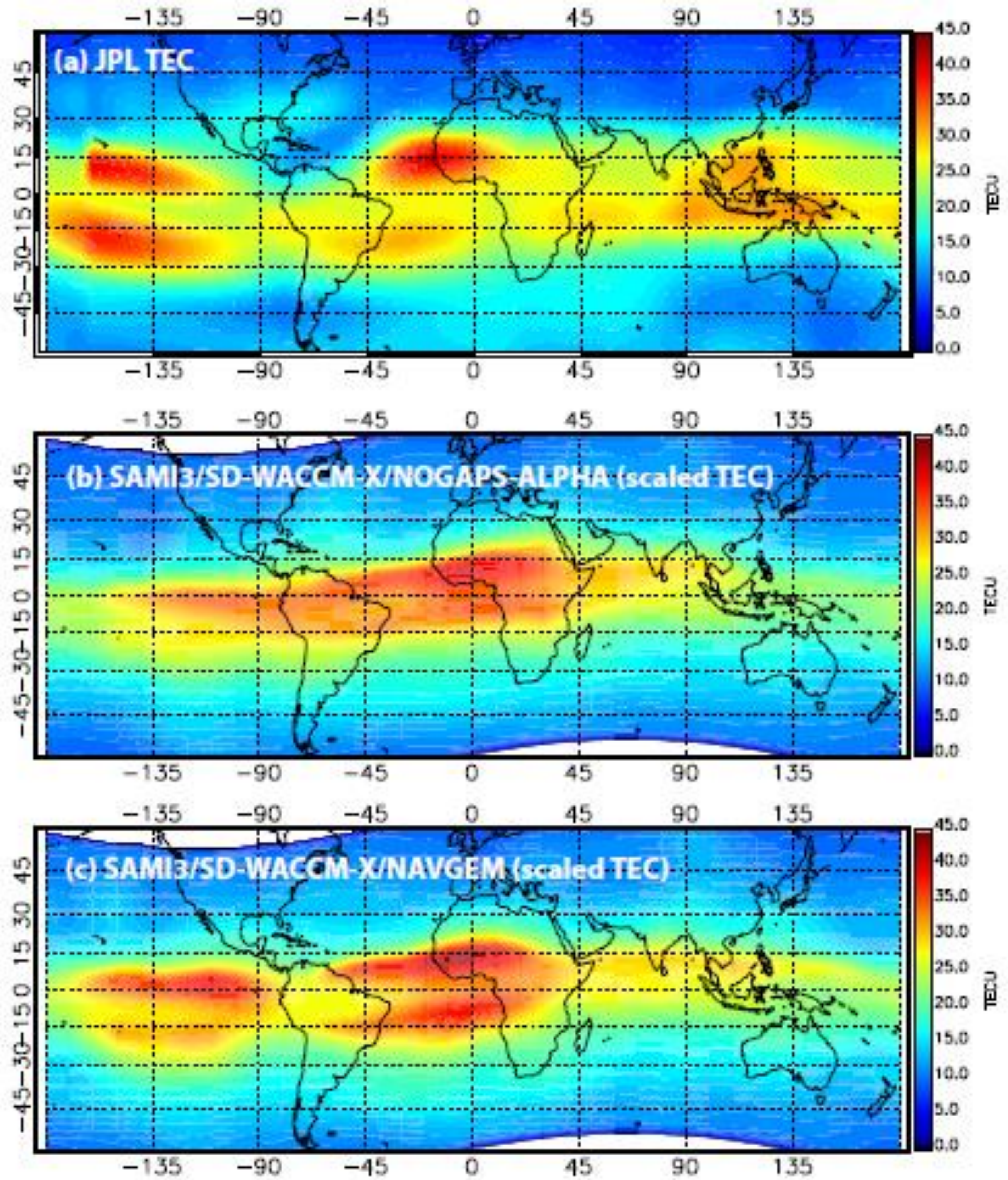

Figure 1.
(a) JPL global ionospheric map of TEC on 12 January 2010 shown at constant local time of 13:00 LT. (b) /NOGAPS-ALPHA simulation of TEC. (c) NAVGEM simulation of TEC. The simulated TEC is scaled by a factor of 0.7 (from McDonald et al., 2018)

To compound the lack of observations, the instruments that produce many of the upper atmosphere observations used in the DA schemes (e.g. SABER, and MLS, the Microwave Limb Sounder) are well past their nominal mission lifetimes and no follow-on programmes are planned. Furthermore, these instruments only observe up to the lower thermosphere and observations higher in the thermosphere are extremely sparse. The QB50 Cubesat project (e.g Gill et al., 2013) focused on the building and launching of instruments to measure thermospheric neutral density, but with little or no attention given to coordination and reception of data. However the constellation of Cubesats used could be a pathfinder for a future operational observations system, with the critical proviso that this constellation would need to be underpinned by associated systems for near real time data reception and cross-calibration of data. In addition, new data from the Global-scale Observations of the Limb and Disk (GOLD) mission will help address the paucity of thermospheric data. The planned assimilation of GOLD O/N2 observations into WAM could test the assumption that temperature is a key variable for the initialization of upper atmosphere models. Since O/N2 plays a key role as a diagnostic of thermospheric transport, it is possible that future DA schemes could instead use O/N2 as a primary control variable.

Model verification using existing data has proved invaluable. However, there is a need for a consistent model verification strategy, and in particular community-wide agreement on which metrics to compare – this could include basic seasonal variability, tide amplitudes and variability, total electron content and the magnitude of the solar semidiurnal migrating tide. An important consideration is to understand which observations are trusted and therefore should be used to validate model output, and there are benefits in an Intergovernmental Panel on Climate Change (IPCC) style model intercomparison, and a cooperative approach. An example is CMIP5 (Taylor et al., 2012) , in which an agreed set of experiments addressing major gaps in understanding was run using multiple models, and output data were formatted in a common way and made freely available via data portals. Empirical models may not be ideal for use as a level of comparison and we suggest the employment of a more general model comparison system, e.g., as implemented in the International Land Model Benchmarking Project (ILAMB, Collier et al., 2018).

4. Future research directions and activities

Based on the discussions throughout the workshop, the following roadmap for future collaboration was agreed:

- Compare existing hydrostatic models to understand impacts of dynamical formulation (also interactions with chemistry, the ionosphere, and radiation)
- Comparison of non-H and hydrostatic dynamical cores to assess impact of non-H cores (and whether non-H is even needed at coarser resolution)
- Assess numerical cost / benefit of comprehensive chemistry schemes designed for climate applications (e.g. WACCM) against simpler schemes designed for near-real time operational use (e.g. as used in WAM)

- Development of a verification strategy and methodology which is required to underpin the above three actions. Clearly, it makes sense to make links with other activities to guide our future actions. These include the Committee on Space Research International Space Weather Action Team and the Community Coordinated Modeling Center (CCMC) Space Weather Modeling Capabilities Assessment (Scherliess et al., 2019)).

Of course, other issues that were discussed at the workshop (such as near real time availability of observations and DA) are very important, but the first focus here is on assessment and developing the whole atmosphere models themselves.

There was a further suggestion that the joint development of parametrizations would be incredibly useful in unifying parametrization strategy across multiple models. The International Space Science Institute has a good setup for accomplishing verification with data, and this setting would be helpful for deciding a verification strategy. To monitor progress, it was also agreed to organize a follow up workshop in mid 2020.

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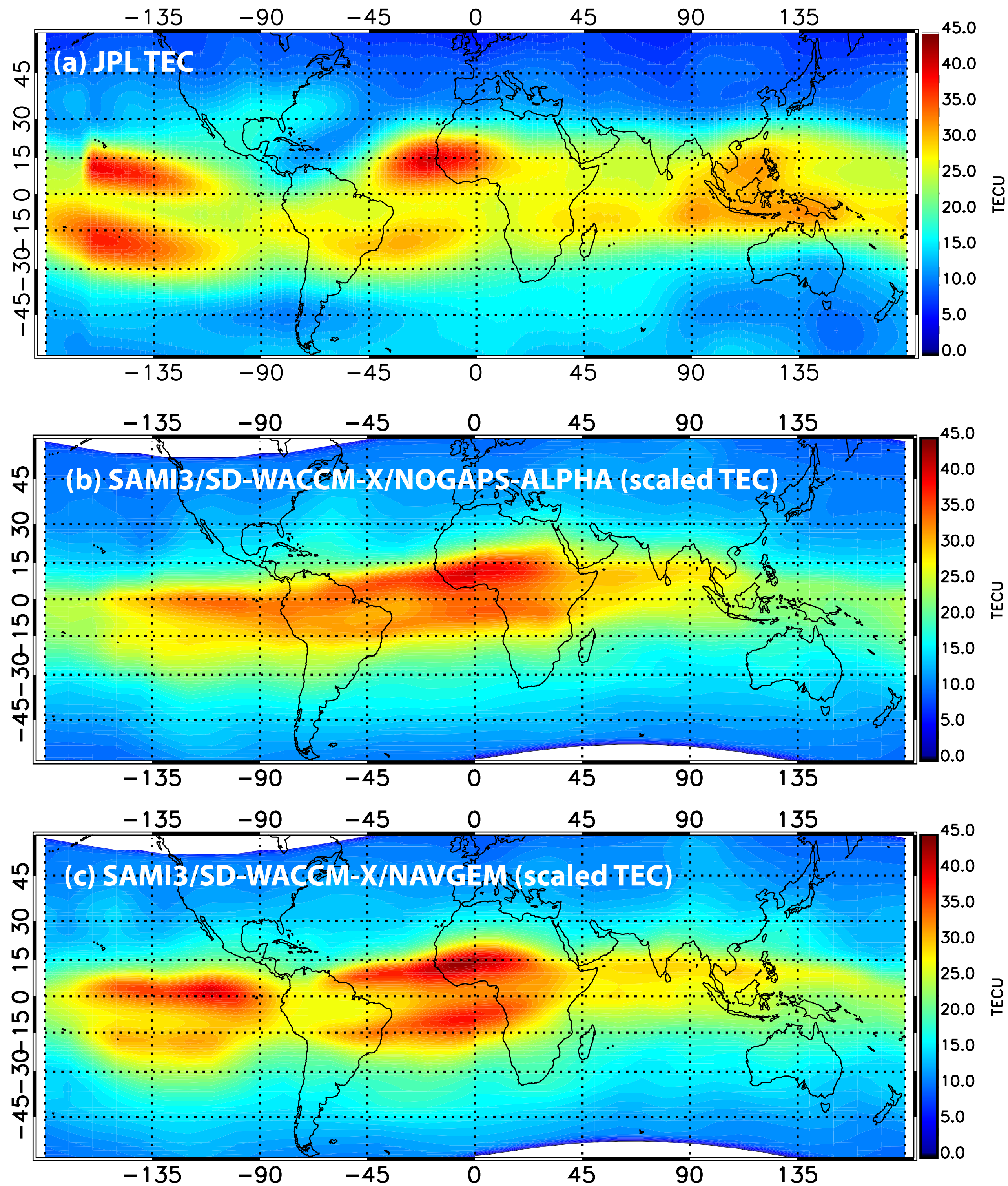

(a) JPL TEC
(b) SAMI3/SD-WACCM-X/NOGAPS-ALPHA (scaled TEC)
(c) SAMI3/SD-WACCM-X/NAVGEM (scaled TEC)
TECU
−135 −90 −45 0 45 90 135
−45 −30 −15 0 15 30 45
0.0 5.0 10.0 15.0 20.0 25.0 30.0 35.0 40.0 45.0