Effects of inferring unobserved thermospheric and ionospheric state variables by using an Ensemble Kalman Filter on global ionospheric specification and forecasting

Chih-Ting Hsu¹, Tomoko Matsuo²,³, Wenbin Wang⁴, and Jann-Yenq Liu¹,⁵

¹Institute of Space Science, National Central University, Jhongli, Taoyuan, Taiwan, ²Cooperative Institute for Research in Environmental Sciences, University of Colorado Boulder, Boulder, Colorado, USA, ³Space Weather Prediction Center, National Oceanic and Atmospheric Administration, Boulder, Colorado, USA, ⁴High Altitude Observatory, National Center for Atmospheric Research, Boulder, Colorado, USA, ⁵National Space Organization, Hsinchu, Taiwan

Abstract This paper demonstrates the significance of ion-neutral coupling to ionospheric data assimilation for ionospheric specification and forecast. Ensemble Kalman Filter (EnKF) is used to assimilate synthetic electron density profiles sampled according to the Formosa Satellite 3/Constellation Observing System for Meteorology, Ionosphere, and Climate into the Thermosphere-Ionosphere-Electrodynamics General Circulation Model (TIEGCM). The combination of the EnKF and first-principles TIEGCM allows a self-consistent treatment of thermosphere and ionosphere coupling in the data assimilation and forecast. Because thermospheric variables affect ionospheric electron densities, different combinations of an observed ionospheric state variable (electron density), and unobserved ionospheric and thermospheric state variables (atomic oxygen ion density, neutral temperature, winds, and composition) are included as part of the EnKF state vector in experiments. In the EnKF, the unobserved state variables are estimated and made dynamically and chemically consistent with the observed state variable, thus improving the performance of the data assimilation system. The impact on ensemble forecast is further examined by initializing the TIEGCM with the assimilation analysis. The main findings are the following: (1) by incorporating ion-neutral coupling into the EnKF, the ionospheric electron density analysis, and forecast can be considerably improved. (2) Thermospheric composition is the most significant state variable that affects ionospheric analysis and forecast. (3) Thermospheric variables have a much longer impact on ionospheric forecast (>24 h) than ionospheric variables (2 to 3 h). (4) In the TIEGCM, the effect of assimilating electron densities is not completely transmitted to the forecast step unless the densities of ion species are estimated.

1. Introduction

The Earth's ionospheric conditions have a significant impact on positioning, navigation and communication systems, and human activities relying on these systems. Therefore, specifying and forecasting the ionospheric conditions accurately are of high relevance to our society. This study is motivated by the need to assess and improve our ability to predict the ionospheric state by taking full advantage of both current numerical models and global ionospheric monitoring techniques.

The ionosphere and thermosphere are a closely coupled system. The state of the ionosphere is greatly influenced by interaction between the neutral and ionized gases. Thus, the thermosphere and ionosphere (T-I) system need to be treated as one coupled system instead of individual independent components. Thermospheric variables can affect ionospheric electron densities through various dynamical, chemical, and electrodynamical processes. In the ionospheric F₂ region, atomic oxygen ions (O⁺) are the dominant ion species. Under the assumption of charge neutrality, in the F₂ region the electron density is nearly equal to the O⁺ density. The variation of the ionospheric electron density can thus be described by the O⁺ continuity equation,

\[
\frac{\partial N}{\partial t} + \nabla \cdot (NV) = P - L
\]  

(1)

where \( N \) is the O⁺ density or electron density, \( V \) is the plasma velocity, and \( P \) and \( L \) are the production and loss rates of O⁺, respectively. The plasma transport processes are represented by the second term on the
left-hand side and the production and loss processes are represented by the terms on the right-hand side. It is evident that the $F$ region electron densities can be affected by neutral winds, temperature, and composition. Neutral winds can change the plasma motion through the collisions between neutrals and charged particles and thereby change electron densities. The $F$ region plasma production and loss processes are largely controlled by neutral composition. The dominant ion production process is the photoionization of atomic oxygen, and the most important loss processes of the plasma is the recombination of molecular ions, as the recombination rate of $\text{O}^+$ is slow. As a result, the neutral atomic oxygen/molecular nitrogen concentration ratio ($\text{O}/\text{N}_2$) is the parameter that largely determines the production and loss in the ionospheric $F_2$ region and the daytime $F_2$ peak density [Rishbeth, 1998]. Moreover, neutral temperature also plays a key role in determining the reaction rate coefficient in the loss process. In most of the ionospheric models, the electron density is equal to the total number densities of all ion species under the assumption of charge neutrality in the ionosphere, while the densities of ion species are obtained either by assuming chemical equilibrium or by solving the ion continuity equation (1) when the life time of a particular ion species, for instance $\text{O}^+$, is long, so transport becomes important [e.g., Richmond et al., 1992; Pi et al., 2003; Schunk et al., 2004]. The continuity equation of $\text{O}^+$ shows, as an example, that the T-I system is not only affected by the momentum and energy deposition due to large-scale wave forcing from below (tides and planetary waves) and solar and magnetospheric forcing from above (solar irradiance and geomagnetic activity) but also is related to the preconditioning of the T-I system as the solution to equation (1) that depends on the initial value of the $\text{O}^+$ density [Jee et al., 2007]. To predict the future behavior of the T-I system, we need the best knowledge of the current state of both the ionosphere and thermosphere. Data assimilation has been proven to be an effective approach to optimally combine available global data and a state-of-the-art, physics-based numerical model to specify the current states of the geophysical system, and for initializing a forecast model of the system [e.g., Daley, 1991; Kalnay, 2003].

Several ionospheric data assimilation models have been developed over the past decade. There are two main ionospheric data assimilation systems that were independently developed by the Utah State University and the team of the University of Southern California and the Jet Propulsion Laboratory [e.g., Pi et al., 2003; Hajj et al., 2004; Schunk et al., 2004; Scherliess et al., 2009]. The physics-based models that were used in these two data assimilation systems are standalone ionospheric models that use an empirical thermospheric model and thus do not include the coupling between the thermosphere and ionosphere. Recently, Matsuo and Araujo-Pradere [2011] used the Ensemble Kalman Filter (EnKF) to assimilate electron density data into a coupled model of the thermosphere and ionosphere which includes the thermospheric feedback on the ionosphere. However, the contribution of each state variable to the assimilation and forecast was not discussed in their study. In this paper, we will use the same EnKF data assimilation system as that of Matsuo and Araujo-Pradere [2011] to study in detail the impact of the coupling between the thermosphere and ionosphere on the ionospheric assimilation and forecast. One of the important assumptions in the EnKF is that the model forecast uncertainty is well emulated by an ensemble of model forecasts. The thermosphere and ionosphere is a dissipative and strongly forced system, highly sensitive to external drivers from which much of the coupled thermosphere-ionosphere model uncertainty originates.

In this study, we will quantify the significance of estimating unobserved thermospheric and ionospheric state variables to ionospheric assimilation and forecast by analyzing the results of seven ensemble experiment. In these ensemble experiments, Observing System Simulation Experiments (OSSEs) are carried out by assimilating synthetic observations sampled from a “true” state according to a realistic observing system into the model. Different combinations of the ionosphere and thermosphere state variables (electron density, atomic oxygen ion density, neutral temperature, winds, and composition) are employed as the EnKF state vector to investigate the impact of estimating unobserved state variables on the performance of the assimilation system. After state variables are initialized by the assimilation analysis of OSSEs, the system is further run without doing any other assimilation to examine the ensemble forecast. The results of seven experiments are compared to the known true state so that the performance of the assimilation system is assessed, and the unobserved variables that have the most significant impact are determined. Thus, this research for the first time systematically and self-consistently evaluate the effect of integrating T-I coupling into data assimilation on the nowcast and forecast of the ionosphere.
The OSSEs are designed according to sampling patterns of the Formosa Satellite 3/Constellation Observing System for Meteorology, Ionosphere, and Climate (FORMOSAT-3/COSMIC) radio occultation electron density profiles. The FORMOSAT-3/COSMIC is a constellation system of six microsatellites that were launched on 15 April 2006 and reached 800 km around December 2007. Each satellite carries four receivers which can receive global position system navigation signals that are transmitted through the ionosphere. Electron density profiles are retrieved from the phase difference of the signals under the assumption of the spherical symmetry of the electron density distribution [Liou et al., 2007]. The large amount of FORMOSAT-3/COSMIC data provides a global coverage of the ionosphere and an unprecedented opportunity to study the global ionospheric specification and forecast by means of data assimilation.

This paper is organized as follows. Section 2 describes the data assimilation system used in this study, including the model and the assimilation techniques. Section 3 describes the design of seven ensemble experiments. Section 4 presents the assimilating and forecasting results obtained from the experiments. Section 5 discusses our results, and the conclusions are given in section 6.

2. Ensemble Kalman Filter Assimilation System

The EnKF assimilation system employed in this study is constructed with the National Center for Atmospheric Research (NCAR) Thermosphere-Ionosphere-Electrodynamics General Circulation Model (TIEGCM) [Richmond et al., 1992] and the Data Assimilation Research Testbed (DART) [Anderson et al., 2009].

The DART is a community software that facilitates assimilation of different kinds of observations into different numerical models using the EnKF technique. The EnKF is a data assimilation method based on a Monte Carlo approximation of a sequential Bayesian filtering process [e.g., Evensen, 1994, 2009]. In the EnKF, an ensemble of model simulations is used to represent the evolution of probability distribution of the T-I system, which is intended to converge toward a more realistic distribution by assimilating observations. In this paper, the term “a priori” refers to the probability distribution before assimilation and “a posteriori” refers to the probability distribution after assimilation. The EnKF is a recursive filter, consisting of analysis (update) and forecast steps. In the analysis step, by using the cross covariance between the observed and the unobserved variables calculated in the EnKF, the a posteriori state variables included in the EnKF state vector (both observed and unobserved variables) are estimated and each ensemble member is updated. In the forecast step, all state variables, including the updated state variables and the state variables that are not updated in the analysis step, are dynamically evolved in the TIEGCM that solves the coupling between these variables. Thus, the adjustment to the updated state variables made in the analysis step can be propagated forward to affect the TIEGCM forecast.

The TIEGCM is a three-dimensional physics-based model of the global coupled T-I system that numerically solves the governing equations of the dynamics, chemistry, and electrodynamics within the system [Richmond et al., 1992]. The default horizontal resolution of the TIEGCM is 5° × 5° in longitude and latitude. The vertical coordinates are given by pressure levels, which extend from about 97 to 800 km (depending on solar activity) with a half-scale height resolution. In the TIEGCM, the O+ density is determined by solving the ion continuity equation for a given initial distribution of O+ density. Densities of other ion species (N+, N2+, O2+, and NO+) are determined according to chemical equilibrium. The electron density is given as a sum of the densities of all ion species under the assumption of charge neutrality.

Recent studies have shown that the DART/TIEGCM data assimilation system can both increase the global information content and the predictability of the T-I system [Matsuo and Araujo-Pradere, 2011; Lee et al., 2012, 2013; Matsuo et al., 2013]. We will further investigate the impact of estimating unobserved thermospheric and ionospheric state variables by using the DART/TIEGCM data assimilation system on the specification and forecast of the global ionosphere.

3. The Ensemble Experiment

Ensemble experiments presented in this study are made of two parts: the 12 h ensemble assimilation and the 24 h ensemble forecast periods. During the assimilation period, seven OSSEs are carried out. The synthetic electron density data are assimilated into the TIEGCM hourly from 0000 UT to 1200 UT of 8 April 2008. Next, ensemble forecast simulations initialized by the assimilation analysis are run from 1200 UT of 8 April through
driven by solar 10.7 cm radio flux ($F_{10.7}$), cross-tail potential drop (CP), auroral hemispheric power (HP), migrating diurnal tides, and semidiurnal tides, and compared to the modeled and observed variability of the ionosphere. The result shows that the effect of $F_{10.7}, HP,$ and CP on the ionospheric electron density is larger than that of tides. Therefore, in this study, the ensemble members are generated by perturbing these three primary input parameters of the TIEGCM: the $F_{10.7}, HP,$ and CP, according to a Gaussian distribution with the assumption of a small systematic bias. $F_{10.7}$ represents the solar Extreme Ultraviolet level that determines the photoionization rates, photodissociation rates, and heating rates of the neutral and ionized species in the model. HP and CP indexes represent the magnitude of auroral particle precipitation and the ionospheric convective electric fields imposed by the magnetosphere. The mean values of the Gaussian distributions for $F_{10.7}, HP,$ and CP are $69 \times 10^{-22} \frac{W}{m^2}, 45$ GW, and $16$ kV, respectively. The corresponding standard deviations for these parameters are set to $5 \times 10^{-22} \frac{W}{m^2}, 10$ GW, and $2$ kV, respectively. Note that CP and HP are correlated to each other so they are not independent parameters. These perturbed input values correspond to geomagnetically quiet conditions for all ensemble members. The spin-up time for model ensemble members is 18 days from 0000 UT of 21 March to 0000 UT of 8 April. The forecast model (a priori) covariance is localized by using the Gaspari and Cohn [1999] function with a half width of 0.2 rad in the horizontal plane and other settings in the TIEGCM and DART are the default values. During both assimilation and forecast periods, model forcing parameters of all ensemble experiments are held unchanged.

A subset of the TIEGCM state variables is selected as part of the EnKF state vector. Different combinations of the ionospheric and thermospheric state variables, including the observed electron density and unobserved atomic oxygen ion density, neutral temperature, zonal and meridional neutral wind velocities, and atomic and molecular oxygen mass mixing ratios, are employed in these seven OSSEs, as summarized in Table 1. A given type of the TIEGCM state variable defined on the model grid is denoted by the vectors $f_e, f_{O}, f_{O}, f_{i}, f_{i}, f_{i}, f_{O}$ and $f_{O}$, representing electron density, atomic oxygen ion density, neutral temperature, zonal and meridional neutral wind velocities, and atomic and molecular oxygen mass mixing ratios on the model grid, respectively. The sum of mass mixing ratios of the major neutral species of the thermosphere (atomic oxygen, molecular oxygen, and molecular nitrogen) is set to equal one in the TIEGCM; hence, the nitrogen mass mixing ratio is also affected when $f_{O}$ and $f_{O}$ are included in the EnKF state vector.

Table 1. List of the State Variables Included in the EnKF State Vector for Each Experiment

<table>
<thead>
<tr>
<th>Experiment</th>
<th>EnKF State Vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$x = [f_e]$</td>
</tr>
<tr>
<td>2</td>
<td>$x = [f_e, f_{O}]$</td>
</tr>
<tr>
<td>3</td>
<td>$x = [f_e, f_{O}, f_i]$</td>
</tr>
<tr>
<td>4</td>
<td>$x = [f_e, f_{O}, f_i, f_i, f_{i}, f_{O}]$</td>
</tr>
<tr>
<td>5</td>
<td>$x = [f_e, f_{O}, f_i, f_i, f_{i}, f_{O}, f_{O}]$</td>
</tr>
<tr>
<td>6</td>
<td>$x = [f_e, f_{O}, f_i, f_i, f_{i}, f_{i}, f_{O}, f_{O}]$</td>
</tr>
<tr>
<td>7</td>
<td>$x = [f_e, f_{O}, f_i, f_i, f_{i}, f_{i}, f_{O}, f_{O}, f_O]$</td>
</tr>
</tbody>
</table>

The impact of including different variables into the EnKF state vector is probed within the framework of TIEGCM physics. Experiment 1, in which only $f_e$ is updated, and Experiment 2, in which both $f_e$ and $f_{O}$ are updated, are compared to examine how the impact of the adjustment of ionospheric state variables in the analysis step is propagated to the forecast step. Because neutral temperature, winds, and composition can significantly affect ionospheric electron densities via transport, production, and loss processes, in Experiment 3, 4, and 5 we not only update $f_e$ and $f_{O}$, but also update unobserved neutral state variables $f_i, f_i, f_i, f_i, f_O$, and $f_O$ separately to incorporate T-I coupling into the analysis step. This allows us to study the influence of T-I coupling on data assimilation. Notice that as mentioned above, by updating $f_O$ and $f_O$, the nitrogen density is effectively updated as well. Experiment 6 updates thermospheric and ionospheric state variables that include observed $f_e$ and unobserved $f_O, f_i, f_i, f_i, f_i, f_O$, and $f_O$. Moreover, Experiment 7, in which $f_e, f_i, f_i, f_i, f_i, f_i, f_O$, and $f_O$ are updated, is compared with Experiment 6 to further investigate the performance of data assimilation system by updating $f_O$ when the neutral state variables are included in both experiments. In addition, the impact of a self-consistent treatment of T-I coupling on the data assimilation is investigated by comparing the results obtained from assimilation experiments that only update ionospheric state variables (Experiments 1 and 2) and those that update both ionospheric and thermospheric state variables (Experiments 3–7).
The data used to conduct OSSEs are synthetic electron density profiles that are based on the geometry of FORMOSAT-3/COSMIC radio occultation events. The synthetic data are generated by sampling a true run of the TIEGCM at the locations of FORMOSAT-3/COSMIC electron density profiles and by adding the observation error. The $F_{10,7}$, HP, and CP values in the true TIEGCM simulation are specified as $74 \times 10^{-22}\ \text{W m}^{-2}\text{Hz}^{-1}$, 55 GW, and 18 kV, respectively. These values, which lie within 1 standard deviation from the mean of Gaussian distributions of respective parameters, make the ensemble TIEGCM simulations biased from the true state. Synthetic electron density profiles are sampled from 160 to 450 km with a vertical resolution of 10 km. The observation error applied to the synthetic electron density profile data is the sum of a 10% instrumentation error and the estimated Abel inversion error percentage [Liu et al., 2010; Yue et al., 2010]. The assimilation window is set to 1 h. The electron density profiles within 30 min before and after a given hour are assimilated for each assimilation cycle. The same synthetic data are assimilated into the TIEGCM in all OSSEs and the performance of the data assimilation system is assessed by the magnitude of the difference between the ensemble mean and the true state.

4. Results

4.1. Ensemble Assimilation Period

The root-mean-square error (RMSE) of $f_{\text{s}}$ is used as the measure of the assimilation analysis accuracy. The RMSE is defined as the root-mean-square difference between the true state, $f^t$, and the ensemble mean, $f^o$, and can be described by

$$\text{RMSE} = \sqrt{\frac{\sum_j (f^o_j - f^t_j)^2}{J}}$$

where $J$ denotes the number of model grid points over a particular region. For cross comparisons, a control experiment is also carried out in which all ensemble TIEGCM simulations are run for the same time period as the OSSEs but without assimilation. Figure 1 displays the a priori and a posteriori RMSEs of Experiment 6 and the RMSEs of control experiment with a 4 h interval during the 12 h assimilation period. The RMSEs at each longitude and latitude location shown in Figure 1 is derived from the corresponding vertical model profiles, so $J$ is equal to the number of model vertical levels. Overall, this OSSE shows that the accuracy of the simulated global electron density distribution becomes closer to the true state by assimilating the synthetic electron density profiles into the DART/TIEGCM data assimilation system. Generally, the reduction of RMSEs of Experiment 6 becomes greater over the assimilation cycles and is evident in the vicinity of most of the observation locations which are indicated by the white dots in Figure 1, especially in the equatorial ionospheric anomaly region.

Figure 2 displays the RMSEs of $f_{\text{s}}$ that were obtained from the results of seven OSSEs and control experiment over the course of the 12 h assimilation period. To obtain a global measure, the RMSE at each time step shown in Figure 2a is derived from global electron densities using all model grid points, so $J$ in equation (2) is equal to the total number of model grid points. To compare the results of ensemble TIEGCM simulations with and without data assimilation, the ratios of the RMSE of OSSEs to the RMSE of the control experiment, referred as the RMSE ratio, are shown in Figure 2b. The RMSE ratio is defined as

$$\text{RMSE ratio} = \sqrt{\frac{\sum_j (f^o_j - f^t_j)^2}{J}} / \sqrt{\frac{\sum_j (f^c_j - f^t_j)^2}{J}}$$

where $f^c$ denotes the mean of control ensemble TIEGCM simulations. Generally, the a priori RMSE (circle symbols) is reduced significantly after assimilation in the analysis step to the a posteriori RMSE (square symbols) and becomes larger in the forecast step (from the a posteriori RMSE to the a priori RMSE of the next assimilation cycle). The RMSEs tends to decrease over all assimilation cycles. Furthermore, the reductions of RMSE in the analysis step of the first assimilation cycle are similar among all OSSEs, but the rate of RMSE growth in the forecast step during the first assimilation cycle is considerably different. This suggests that the impact of updating unobserved variables primarily manifests in the forecast steps. In the forecast step, state variables that are updated in the analysis step influence the $O^+$ and electron density calculation through the T-I coupling processes described in the TIEGCM.

In Experiment 1, the a posteriori RMSEs are reduced from the a priori RMSEs after assimilation (blue circle and squares in Figure 2). However, the a priori RMSEs immediately go back to the same level as that of the
RMSEs of the control experiment over an assimilation cycle. This result suggests that the influence of data assimilation is lost over just one assimilation cycle when the EnKF state vector is composed only of \( f_e / C_0 \). In other experiments, on the other hand, the error reduction due to data assimilation is propagated to and accumulated over subsequent assimilation cycles. In Experiment 2 the a priori and a posteriori RMSEs (red circles and squares) decrease in the first two assimilation cycles and then become almost constant. The comparison of Experiments 1 and 2 implies that when the unobserved state variable \( f_{O^+} \) is updated along with the observed state variable \( f_e \), the accuracy of the data assimilation analysis is improved globally. In the section 5 we will elaborate upon this behavior of the DART/TIEGCM data assimilation system.

Experiments 3–5 illustrate the impact of updating unobserved thermospheric state variables \( f_T, f_U, f_V, f_O, \) and \( f_{O_2} \) on the RMSEs of \( f_e \) (green, cyan, and orange symbols). It can be seen that updating these thermospheric state variables can reduce both the a priori and a posteriori RMSEs and thereby improve the performance of the data assimilation system even though these thermospheric state variables are not observed. In the EnKF, the unobserved state variables are estimated by using the cross covariance between the unobserved state variables and the observed state variables. Therefore, the unobserved thermospheric state variables become dynamically and chemically more consistent with the observed variable (electron density) of the ionosphere, as well as the a posteriori RMSEs are reduced. On the other hands, in the forecast step, the adjusted observed and unobserved variables propagate forward. This kind of adjustment further affects the state variables that are not included in the EnKF state vector and impacts the a priori RMSEs. At the beginning of the 12 h assimilation period (from 0000 UT to 0200 UT), the a posteriori RMSEs of Experiments 4 and 5 are similar with each other, and the a posteriori RMSEs of Experiment 3 are the largest of these three experiments. However, the growth of RMSE during the forecast step appears to be slower in Experiment 5 than those in Experiments 3 and 4.

**Figure 1.** The root-mean-square errors (RMSE) of the electron density in latitude-longitude coordinate during 12 h ensemble assimilation period. (top, middle, and bottom) The RMSEs of the control experiment, and those of a priori and a posterior for Experiment 6, updating \( f_e, f_{O^+}, f_T, f_U, f_V, f_O, \) and \( f_{O_2} \), respectively. From left to right panels are the RMSEs at 0000 UT, 0400 UT, 0800 UT, and 1200 UT, respectively. White dots display the trajectory of assimilated synthetic electron density profiles.
The end of the 12 h assimilation period, the a posteriori RMSEs of Experiment 5 decrease from 86% at 0000 UT to about 38% at 1200 UT of the RMSEs of the control experiment, which is smaller than those of Experiments 3 (43%) and 4 (46%). Thus updating $f_{O_2}$ in the EnKF is more effective at improving the ionospheric electron density analysis than updating $f_T$, $f_U$, and $f_V$.

The decrease of the RMSEs in Experiment 7, which does not include $f_{O_2}$ in the EnKF state vector, is generally smaller than those of the experiments that have $f_{O_2}$ in the EnKF state vector (Experiments 2–6) over the entire course of the assimilation period. This result, along with that obtained by comparing Experiments 1 and 2 in the previous paragraph, shows that updating $f_{O_2}$ in the assimilation period is important even though it is not an observed ionospheric state variable. Furthermore, it is interesting to note that the RMSE values of

![Figure 2](image-url).

This figure shows the a priori and a posteriori global mean (a) RMSEs and (b) RMSE ratios of the electron density during 12 h ensemble assimilation period (from 0000 UT to 1200 UT of 8 April 2008). The gray solid lines denote the RMSEs and RMSE ratios of the ensemble simulation without assimilation (control experiment). Circles and squares represent the values of a priori and a posteriori RMSEs and RMSE ratios, respectively.
Experiments 5 and 6 are very close over the entire assimilation period, which again suggests that thermospheric composition $f_{O}$ and $f_{O2}$ are the most important neutral parameters in determining the performance of the ionospheric data assimilation system.

4.2. Ensemble Forecast Period

The geophysical conditions (including $F_{10.7}$, HP, and CP) to drive the TIEGCM are held unchanged over the assimilation and forecast periods in this study. Because TIEGCM ensemble simulations are synthetically biased from the true state which synthetic observation are sampled, we can study how fast the TIEGCM state variables return to the control state that is solely controlled by the model forcing parameters after being modified by data assimilation and which neutral and ionospheric state variables are the critical one that determine this recovery. The rate of recovery to the control state depends on the time scale of the production, loss, and transport processes, as well as the initial values of the state variables. In the forecast period, seven ensemble forecast experiments are conducted to examine the rate at which the ionospheric state goes back to the control state in the TIEGCM after thermosphere and ionospheric state variables are initialized by the assimilation analysis of the corresponding OSSEs of assimilation period. The relative importance of different T-I coupling processes on the ionospheric forecast is assessed by comparing results of ensemble forecasting experiments.

Figure 3 displays the global RMSEs of $f_i$ computed from the results of seven sets of ensemble forecast simulations which are initialized by the analysis of corresponding experiments described in section 4.1. The global RMSEs of an additional set initialized with control ensemble experiment are also performed in Figure 3. The RMSE and RMSE ratio shown in Figures 3a and 3b are computed in the same way as for Figures 2a and 2b. In general, the rate of reversion, as represented by the RMSEs of these experiments, is slower in Experiments 3–7, in which both thermospheric and ionospheric state variables are initialized, than in Experiments 1 and 2, in which only the ionospheric state variables are initialized. This means that the effect of initializing both ionospheric and thermospheric state variables on the ionospheric forecast lasts longer, due to the fact that the thermosphere has a longer memory in comparison with the ionosphere [Jee et al., 2007, 2008]. Thus, the thermospheric variables initialized by the assimilation analysis modify the electron densities through the T-I coupling processes over the course of the entire forecast period.

At the beginning of the 24 h ensemble forecast period, the RMSE of Experiment 1 is about 65% of the RMSE of the control experiment, but the effect of the assimilation is lost in just 1 h. This behavior is consistent with the result of Experiment 1 shown in Figure 2. On the contrary, other forecast experiments behave considerably differently. The RMSE of Experiment 2 is about 48% of the RMSE of the control experiment at the beginning of forecast period. Then it rises to about 70% 1 h later and slowly approaches to 97% of the RMSE of the control simulation over the course of 10 h. The forecast result of Experiment 2 illustrates that the impact of
 initializing the TIEGCM with the assimilation analysis of the ionospheric state variables ($f_e$ and $f_{O^+}$) is mostly lost in about 2 to 3 h and almost completely lost after about 12 h.

The RMSEs of Experiments 3–5 in the forecast step increase to about 86%, 89%, and 68% of the RMSE of the control experiment after 6 h, to about 90%, 96%, and 75% after 12 h, and to 98%, 99%, and 79% after 24 h, respectively. These experiments demonstrate that the impact of data assimilation can be sustained longer than 24 h in the forecast of the TIEGCM if neutral state variables are continuously updated in the analysis step of the EnKF and the results are employed as the initial values for forecast. Moreover, neutral composition ($f_O$ and $f_{O_2}$), which can affect ionization and recombination rates in the chemical processes on the ionosphere and consequently change the ionospheric electron density, is the most significant neutral state variable that affects the performance of the TIEGCM forecast.

Results of Experiments 6 and 7 reflect the fact that the thermosphere has a longer memory than the ionosphere. Although the RMSE values of Experiment 7 are larger than that of Experiment 6 at the beginning of the forecast period (1200 UT), the RMSEs of these two experiments become almost identical after 10 h in the forecast period. The impact of initialization persists longer than 24 h in both Experiments 6 and 7, as the RMSEs from these two experiments are still about 80% of that of the control experiment. The comparison of Experiments 6 and 7 shows that initialization of the TIEGCM with the assimilation analysis of the ionospheric state variables improves the predictability of the ionosphere within first 10 h of the forecast, but initialization of the model with the assimilation analysis of the thermospheric state variables has a much longer impact on the ionosphere forecast. As a consequence, the RMSE of the forecast is relatively small for more than 10 h if we update thermospheric state variables in the assimilation period.

Furthermore, the comparison of RMSEs from all ensemble forecast experiments shows that $f_O$, $f_{O_2}$, and $f_{O^+}$ are the major physical parameters that determine the performance of the forecast. It is thus critical in the ionosphere data assimilation to include them in the state vector and update them continuously during the assimilation cycles, even though these variables may not be observed.

5. Discussions

In the EnKF experiments with the DART/TIEGCM presented in Matsuo and Araujo-Pradere [2011], different combinations of $f_e$, $f_T$, $f_U$, $f_V$, $f_O$, and $f_{O_2}$ were also included in the state vector to study the role of thermosphere-ionosphere coupling in the coupled thermosphere-ionosphere data assimilation and its impact on global ionospheric specification. Although the contribution of each variable is not discussed in detail in that study, their conclusion is essentially consistent with our findings. Updating both ionospheric and thermospheric state variables in the EnKF can more greatly improve the ionospheric specification than updating the ionospheric state variable $f_e$ alone.

By replacing the initial condition of the electron density field in a coupled T-I model with an electron density field that was generated by an ionospheric data assimilation system, Jee et al. [2007, 2008] studied how long the initial conditions continue to influence the ionosphere and the effect of the ionospheric plasma density changes on the thermosphere. Their results show that the e-folding time of initializing the ionospheric part of the coupled T-I model is about 2 to 3 h. This is due to the fact that chemical process is one of the dominant processes that determine the ionospheric plasma densities near the $F_2$ peak. The effect of the adjustment of the plasma density quickly disappeared as the thermosphere state, especially composition, did not change adequately to be consistent with the imposed ionospheric initial conditions in this case. Basically, the thermosphere was initialized with the climatological model state so that the ionosphere was forced back to the climatological model state through, mostly, ion-neutral chemical process. This is also consistent with our Experiments 1 and 2. The lifetime of $O^+$ is about 2 h, and therefore, both Jee et al. [2007, 2008] and our results are very much in align with this time constant.

On the other hand, during the 24 h ensemble forecast period of our Experiments 3 to 7 both the ionosphere and thermosphere are initialized with the best estimation of the updated ionospheric and thermospheric state variables when the thermospheric state variables was also updated during the 12 h ensemble assimilation period. Thus, the effect of only adjusting ionospheric state variables last relatively shorter than that of adjusting both ionospheric and thermospheric state variables. Furthermore, unlike the $F$ region ionosphere, which has a relatively short lifetime of about 2 h, changes to thermospheric variables take much longer time to recover.
[e.g., Burns et al., 1991]. Thus, the perturbed thermospheric state variables in the assimilation period of Experiment 3 to 7 can affect the simulation results for a considerably long period of time.

Following earlier studies of Jee et al. [2007, 2008], in which the TIEGCM simulations were initialized by the assimilation analysis, Chartier et al. [2013] examine the impact of initializing both ionospheric and thermospheric state variables (including $f_{e}$, $f_{o}$, $f_{r}$, $f_{u}$, $f_{v}$, $f_{O}$, and $f_{O_{2}}$) on the TIEGCM simulations during geomagnetic storms. Their results show that the impact of initializing thermospheric state variables on the ionospheric forecast persists longer than that of ionospheric state variables and that thermospheric composition is the most significant state variables that impacts the ionospheric forecast. In their experiments, the initial model state is replaced with the truth, which is unrealistic from the perspective of data assimilation, although their general findings are consistent with our findings.

In Experiments 3–5, different thermospheric state variables, $f_{r}$, $f_{u}$, $f_{v}$, $f_{O}$, and $f_{O_{2}}$, are updated to assess the impact of inferring neutral temperature, winds, and composition in the coupled thermosphere-ionosphere data assimilation system on the ionospheric specification and forecast. These experiments are conducted under geomagnetically quiet conditions. The results of these experiments shows that to improve both specification and forecast of the global ionosphere, $f_{O}$ and $f_{O_{2}}$ (associated with thermospheric composition) are the most important state variables that need to be estimated in the assimilation period by taking advantage of the T-I coupling. Rishbeth and Edwards [1989] and Rishbeth [1998] show that the ionospheric electron density distribution of the dayside $F$ region is determined mostly by the atomic oxygen/molecular nitrogen concentration ratio under geomagnetically quiet conditions. In the TIEGCM, the sum of the atomic oxygen, molecular oxygen, and molecular nitrogen mass mixing ratios is set to equal 1, and therefore, the nitrogen mass mixing ratio is determined when the rest are known. The adjustment of $f_{O}$ and $f_{O_{2}}$ by the EnKF effectively modifies the ratio of atomic oxygen to molecular nitrogen density, and subsequently the electron density loss and production process in the TIEGCM. The importance of initializing the thermospheric composition to the ionospheric forecast has also been demonstrated for storm cases by Chartier et al. [2013]. Although this study simply investigates the impacts of seven variables under geomagnetic quiet condition, the result shows that state variables with timescale being relatively long are important to determine the electron density, and due to these state variables, the effect of the adjustment of the electron density should also stay longer, even if under different geomagnetic conditions.

In the EnKF, we expect that the performance of our system will become better if more state variables are included as part of the EnKF state vector. However, Figure 2 shows that the RMSEs of Experiment 5 are smaller than that of Experiment 6 in the 12 h ensemble assimilation period, suggesting that this is not necessarily the case. When updating state variables in the EnKF through cross covariance, the estimated state variables might become dynamically inconsistent with each other due to the effect of sampling errors in the sample covariance estimated from a finite number of ensemble members. The effect of sampling errors can be rectified by the use of covariance localization to some extent [e.g., Evensen, 2009], and it needs to be further investigated in the future.

In Experiment 1, the RMSEs of $f_{e}$ are reduced by assimilating the synthetic electron density profiles. However, the effect of adjusting electron densities in the analysis step does not fully propagate to the forecast step unless both $f_{e}$ and $f_{O}$ are updated in the analysis step. This is because the atomic oxygen ion density, instead of the electron density, is the physical field calculated by solving the ion continuity equation (1) in the TIEGCM.

Lee et al. [2012] present the assimilation analysis of electron densities by updating the same state variables as those in Experiment 7. Although their result shows that the specification of the electron density can be improved by assimilating electron density profiles into the DART/TIEGCM system, the a posteriori electron densities exhibited the tendency to relax back toward the climatology very fast. The comparison of the forecast period result of the Experiments 6 and 7 shows the similar behavior. This is related to the fact that during the assimilation period $f_{O}$ is updated in Experiment 6, but not in Experiment 7. As shown in Experiment 2, the impact of updating $f_{O}$ lasts for about 10 h. After that RMSEs of Experiments 6 and 7 are purely determined by the effect of updating neutral variables, and thus, RMSEs become the same.

6. Conclusions

This paper demonstrates the significant effect of updating thermospheric state variables, especially composition, in the coupled thermosphere-ionosphere data assimilation system on both assimilation...
Acknowledgments

The authors sincerely thank Timothy Hoar and Jeff Anderson at the Institute for Mathematics Applied to Geosciences (IMAGe), NCAR for their great help with DART/TIEGCM. We also thank Nicholas Pedatella and Chien-Hung Lin for their helpful comments. The DART software was obtained from IMAGe, NCAR (URL: http://www.image.ucar.edu/DARt/DART/). The TIEGCM were obtained from High Altitude Observatory, NCAR (URL: http://www.hao.ucar.edu/modeling/tgcm/tie.php). The FORMOSAT-3/COSMIC data were obtained from COSMIC Data Analysis and Archival Center (CDAAC) (URL: http://cdaac-www.cosmic.ucar.edu/cdaac/index.html) and Taiwan Analysis Center for COSMIC (TACC) (URL: http://tacc.cwb.gov.tw/). This work is supported by Taiwan Ministry of Science and Technology grant MOST103-2628-M-008-001, Air Force Office of Scientific Research grant FA9550-13-1-0058, and National Aeronautics and Space Administration grants NNX12A534G, NNX13A020G, NNX14A06G, and NNX15AQ99G. NCAR is sponsored by the U.S. National Science Foundation. Simulation data used in this paper may be obtained by contacting the corresponding author, Jann-Yenq Liu.

Alan Rodger thanks the reviewers for their assistance in evaluating the paper.

analysis and forecast of the global ionosphere and serves as guidance to future research and development of global ionospheric data assimilation systems. The National Center for Atmospheric Research Thermosphere-Ionosphere-Electrodynamics General Circulation Model (TIEGCM) and Data Assimilation Research Testbed (DART) are used to assimilate synthetic electron density profiles which are sampled using the geometry of the Formosa Satellite 3/Constellation Observing System for Meteorology (FORMOSAT-3/COSMIC) radio occultation data. In our seven Observing System Simulation Experiments (OSSEs) that are carried out as the ensemble assimilation experiments, different combinations of the thermospheric state variables (winds, temperature, and composition) and the ionospheric state variables (electron density and atomic oxygen ion density) are included as part of the EnKF state vector and the values of these variables are inferred by assimilation of the synthetic electron density profiles. These 12 h ensemble assimilation experiments have been conducted from 0000 UT to 1200 UT of 8 April 2008 using a 90 member ensemble with a 1 h assimilation window. In addition, the 24 h ensemble forecast experiments initialized with the assimilation analysis subsequently carried out from 1200 UT of 8 April through 1200 UT of 9 April.

The main findings of this study are as follows:

1. By including unobserved thermospheric variables (neutral temperature, compositions, and winds) into the state vector of the EnKF assimilation system, the accuracy of ionospheric analysis and forecast is considerably improved.

2. The comparison of data assimilation experiments suggests that the impact of updating neutral composition is greater than updating neutral winds and temperature in the analysis step of the EnKF on the ionospheric specification. This is due to the fact that the daytime ionospheric F2 region electron density is mostly determined by the atomic oxygen/molecular nitrogen concentration ratio under geomagnetically quiet conditions.

3. The comparison of ensemble forecast experiments shows that initialization by using the assimilation analysis of both thermospheric and ionospheric state variables impacts the ionospheric forecast for more than 24 h, which is much longer than the case of initialization of the ionospheric state only (2 to 3 h). Additionally, initializing the ensemble forecast experiment with the assimilation analysis of neutral composition can improve the performance of the data assimilation system by about 20% over 24 h.

4. Because the electron density is given as a sum of the ion species in the TIEGCM, the effect of assimilating electron densities is not completely passed into the forecast step unless the densities of ion species are updated along with the electron density in the analysis step of the EnKF. In the ionospheric models, in which the continuity equations of ion species are solved in a way that is similar to that in the TIEGCM, it is important to update the ion species along with electron densities in the data assimilation.

References


