Design and Preliminary Experiment of the TIEGCM Ensemble Kalman Filter Data Assimilation Model (Postprint)

Authors: Zhang Yanan, Wu Xiaocheng, Hu Xiong

Date: 2017-01-22T00:00:00+00:00

Abstract

This study employs the parameterized ionosphere-thermosphere theoretical model TIEGCM as the background model and develops a global ionospheric electron density assimilation model using the ensemble Kalman filter method based on electron density profile data from COSMIC occultation observations, thereby achieving global ionospheric electron density assimilation. The assimilation results indicate that this model can effectively assimilate observational data into the background model to obtain global three-dimensional ionospheric electron density. Compared with the background model, the deviation of the assimilated electron density relative to observations is significantly reduced. Additionally, a comparison between sequential assimilation and simultaneous assimilation reveals that the improvement in mean bias is essentially consistent, while the standard deviation after simultaneous assimilation exhibits a slight reduction above the peak height.

Full Text

Preamble

TIEGCM Ensemble Kalman Filter Assimilation Model Design and Preliminary Results

ZHANG Yanan[1,2], WU Xiaocheng[1], HU Xiong[1]

[1] National Space Science Center, Chinese Academy of Sciences, Beijing 100190
[2] University of Chinese Academy of Sciences, Beijing 100049

Abstract

This study employs the parameterized ionosphere-thermosphere theoretical model TIEGCM as the background model and establishes a global ionospheric electron density assimilation model using the ensemble Kalman filter method based on COSMIC occultation observation electron density profile data, enabling global ionospheric electron density assimilation. The assimilation results demonstrate that this model can effectively incorporate observational data into the background model to obtain global three-dimensional ionospheric electron density. Compared with the background model, the deviation of assimilated electron density relative to observations decreases significantly. Furthermore, comparison between batch assimilation and simultaneous assimilation reveals that both methods achieve similar improvements in mean bias, while simultaneous assimilation yields slightly reduced standard deviation above the peak height.

Keywords: ionosphere, data assimilation, ensemble Kalman filter, simultaneous assimilation

1 Introduction

The electron density distribution in the ionosphere affects navigation and shortwave communication systems, thereby influencing human activities. The ionosphere varies with longitude, latitude, altitude, local time, season, solar activity, and geomagnetic activity due to internal and external driving factors [1]. Monitoring the ionospheric state through observations alone is difficult because observations lack sufficient spatiotemporal resolution.

Ionospheric models have long been fundamental tools for ionospheric research and forecasting, including empirical and theoretical models. Empirical models, derived from statistical analysis of extensive observational data, can accurately perform medium- and long-term forecasting but struggle with accurate short-term forecasting. Theoretical models, based on physical equations, can perform short-term forecasting. However, because theoretical models cannot comprehensively and accurately account for all physical processes and disturbances in the ionosphere, combined with uncertainties in boundary and initial conditions and numerical method errors, theoretical model forecasts often deviate significantly from actual conditions [2]. Most empirical and theoretical models can simulate ionospheric climatological characteristics but cannot accurately perform ionospheric nowcasting and forecasting due to their lack of reliable estimates of ionospheric driving factors.

To meet the demands of ionospheric monitoring and forecasting, data assimilation techniques—already mature in meteorology—have been introduced to ionospheric research and forecasting. Over the past decade, many ionospheric data assimilation models have been developed based on empirical or theoretical models and various ionospheric observations. Since these models primarily assimilate ground-based observations with limited spatial coverage, they cannot precisely characterize global electron density distribution. However, with the development of GNSS, the spatial coverage of ground-based GNSS-TEC observations and space-based occultation observations has become increasingly extensive. Occultation observations, in particular, provide three-dimensional electron density distributions for oceanic, desert, and polar regions with sparse observations.

International ionospheric data assimilation research began in the last century, with notable examples including the JPL/USC GAIM (Jet Propulsion Laboratory/University of Southern California Global Assimilation Ionospheric Model) and the USU GAIM (Utah State University Global Assimilation of Ionospheric Measurements) [3]. The USU GAIM assimilation model includes both Gauss-Markov Kalman filter and reduced-state Kalman filter assimilation modes [4, 5]. In recent years, foreign scholars have conducted research on ionospheric assimilation, ionospheric driving parameters, and the effects of ionosphere-thermosphere interactions on ionospheric assimilation [6, 7], achieving considerable results. Domestic research in this area remains limited, primarily focusing on Dr. Yue Xin' s work on mid- and low-latitude ionospheric simulation and data assimilation, with his research on ionospheric electron density spatial correlation holding significant value for ionospheric assimilation studies [2].

This paper employs the ensemble Kalman filter assimilation method to assimilate COSMIC electron density profiles into the TIEGCM model developed by NCAR, presenting preliminary results and further discussion, while comparing two assimilation approaches.

2.1 Ensemble Kalman Filter Method

Evensen et al. [8] proposed a Monte Carlo random sampling-based Kalman filter method known as the Ensemble Kalman Filter (EnKF). Compared with variational methods and the Kalman filter, EnKF uses finite samples from nonlinear ensemble forecasts to estimate error covariance, making it applicable to highly nonlinear dynamic models without requiring tangent linear operators, adjoint equations, or backward time integration. The basic filter formulas are:

$$P^e = X' X'^T$$
$$K = P^e H^T (H P^e H^T + R^e)^{-1}$$
$$X^a = X^b + K(Y - HX^b)$$

where X' is the background perturbation field, P^e is the background error covariance matrix, and R^e is the observation error covariance matrix. K is the gain matrix used to correct the background field near observation points. X^b is the background field, Y is the observation vector, H is the observation operator, and X^a is the assimilation result. EnKF uses sample statistics to calculate background error covariance, which can produce spurious false correlations, requiring correlation distance control through covariance localization.

2.2 Assimilation Variable Configuration

Equation (3) shows that assimilation requires the background field X^b, observations Y, the interpolation or observation operator H mapping from background field to observations, and the error covariance matrices P and R for background field and observations. The acquisition of these quantities is described below.

The background field is obtained from TIEGCM model forecasts. The TIEGCM [7] developed by NCAR is a three-dimensional, time-dependent, coupled Earth thermosphere-ionosphere theoretical model. Using finite difference techniques, it self-consistently solves three-dimensional momentum, energy, and continuity equations for neutral components and ions. Its default resolution is 5 degrees in longitude and latitude, with 29 layers in the vertical direction at half-scale height intervals. The lower boundary is approximately 97 km, while the upper boundary varies between 500 km and 700 km depending on solar activity.

TIEGCM is an ionosphere-thermosphere electrodynamic general circulation model that forecasts many atmospheric parameters, including electron density and atmospheric temperature. Data from day 80 of 2006 is selected as the initial value, with model forecasts run to 00:00 UT on day 159. The solar activity index F10.7 in the model input parameters is then perturbed to construct an ensemble of 100 samples with a mean of 150 and standard deviation of 50%. These 100 samples serve as input parameters to the model, which forecasts for 6 hours to obtain the background field X^b.

Observations are COSMIC occultation electron density profile data. The COSMIC occultation electron density profile data used here are Level 2 ionospheric data products provided by UCAR. Research shows that due to the spherical symmetry assumption in Abel inversion, electron density retrieval results below the F-region should be used with caution [9]. Therefore, this study only assimilates electron density above 150 km with an interpolation grid spacing of 10 km. Observational data from around 06:00 UT on day 159 of 2007 (within half an hour) are used as the observation field. For quality control, observations with values greater than zero are retained. After preliminary quality control, approximately 3,580 observation points from 121 profiles remain.

TIEGCM outputs grid heights as geopotential heights. To facilitate construction of the observation operator, geopotential height is converted to geometric height and interpolated to constant geometric height surfaces. The observation operator uses spatial linear interpolation within the grid cube containing the observation point.

The background field error covariance is obtained from ensemble sample statistics. In most assimilation systems, observation errors are assumed to be independent [10, 11]. This study adopts the same assumption, neglecting observation covariances and assuming observation bias to be 20% of the observation value. The observation error covariance is:

$$R = \begin{cases} 0.04 \times y_i \times y_i, & i = j \\ 0, & i \neq j \end{cases}$$

2.3 Localization

In the ensemble Kalman filter method, finite ensemble size causes rank deficiency and spurious correlation noise. To eliminate false correlations far from observations, covariance localization is required. Ionospheric spatial correlation is generally assumed to follow a Gaussian distribution, though no definitive conclusion exists regarding correlation distance [12]. Ionospheric correlation distance can be considered anisotropic. Here, ionospheric correlation is simply decomposed as the product of meridional, zonal, and vertical components [2]. Ionospheric correlation scales differ significantly across directions and exhibit clear variations with latitude, altitude, local time, season, and solar activity. Vertical correlation distance increases with altitude, with upward correlation distance greater than downward correlation distance. Overall, zonal correlation distance is larger than meridional correlation distance.

Multiplying the background error covariance estimated from ensemble samples with the localization correlation function yields a new covariance matrix:

$$\rho_{ij} = e^{-\alpha \times (\varphi_{ij}^2)} \times e^{-\alpha \times (\theta_{ij}^2)}$$
$$P'_{ij} = \rho_{ij} \times P_{ij}$$

where ρ_{ij} is the correlation coefficient between points i and j, and φ_{ij} and θ_{ij} represent the actual distances between the two points in longitude and latitude directions. Defining the correlation distance as the distance where the correlation coefficient between two points equals 0.75, and based on Yue Xin et al. [2], the latitudinal correlation distance L_x is taken as 10°, the longitudinal correlation distance L_y varies from ~40° at mid-latitudes to ~20° at the equator, and vertical correlation is set as uncorrelated. α is the correlation distance coefficient, where $0.75 = e^{-\alpha}$ gives $\alpha = 0.2877$.

2.4 Assimilation Methods

Sequential assimilation assimilates observation data one by one, while simultaneous assimilation assimilates all observation data at once. Sequential assimilation represents local optimization for observation data, whereas simultaneous assimilation represents global optimization for all observation data. Research shows [13] that when observation errors are uncorrelated, the difference between sequential and simultaneous assimilation in ensemble Kalman filtering is minimal. Sequential assimilation assimilates only one observation at a time, requiring less computer memory but taking longer to assimilate all observations. Simultaneous assimilation assimilates all observations at once, offering higher computational efficiency but requiring larger computer memory. When the amount of assimilated data is large, memory requirements may exceed computational capacity. Combining the advantages of both methods leads to batch assimilation, where observations are assimilated in groups.

To compare differences between batch assimilation and simultaneous assimilation, this study performs assimilation using both methods and compares the results. For batch assimilation, observations are assimilated profile by profile.

3.1 Assimilation Results

Fifty percent of the 121 observation profiles are randomly selected for assimilation using simultaneous assimilation, with the remaining 50% of unassimilated profiles used to validate assimilation effectiveness. Results are presented below.

[Figure 1: see original paper] Comparison of electron density profiles between background (dashed lines) and EnKF-assimilated (solid lines) fields for assimilated observations (dash-dotted lines).

[Figure 2: see original paper] Comparison of electron density profiles between background (dashed lines) and EnKF-assimilated (solid lines) fields for unassimilated observations (dash-dotted lines).

Examples comparing assimilation results with observations and pre-assimilation background fields are provided, where dark gray dash-dotted lines represent observations, light gray dashed lines represent the background field, and black solid lines represent the analysis field. The background and analysis field profiles used for comparison are interpolated to corresponding observation points. The results show that in Figure 1, the analysis field is much closer to observations. In Figure 2, although these observation profiles were not assimilated, the analysis field still agrees better with observations due to correlations provided by the background field. This demonstrates that the assimilation model can effectively incorporate observational data into the background model to obtain a global three-dimensional ionospheric electron density analysis field, providing good improvement even in locations without observational data.

3.2 Relative Error

To further validate assimilation effectiveness, statistics of background field and assimilation results relative to observations are calculated at different altitudes. The formulas for relative error, mean bias, and standard deviation are:

$$e_i = \frac{x_i - y_i}{y_i} \times 100\%$$

$$\sigma_x = \sqrt{\overline{(e_i - \bar{e})^2}}$$

where x_i is the background field or assimilation result at a location, y_i is the corresponding observation, e_i is the relative error of electron density, and $\bar{e}$ and σ_x are the mean bias and standard deviation of relative electron density error at the corresponding altitude.

[Figure 3: see original paper] Statistical distribution of electron density error at observation profiles used in assimilation before (left) and after (right) simultaneous assimilation.

[Figure 4: see original paper] Statistical distribution of electron density error at observation profiles not used in assimilation before (left) and after (right) simultaneous assimilation.

[Figure 5: see original paper] Profile of relative standard deviation of background field samples at 115°E, 40°N.

In Figures 3 and 4, solid lines in the left panels show the mean bias of the pre-assimilation background field, with dashed lines representing mean bias plus/minus one standard deviation. Right panels show error statistics for the post-assimilation analysis field. The results indicate that for both assimilated and unassimilated observation profiles, the mean bias and standard deviation of the analysis field are generally reduced compared to the pre-assimilation background field. Above 300 km, the mean bias decreases from 50% pre-assimilation to within 15% post-assimilation, while the standard deviation decreases from above 50% pre-assimilation to within 40% post-assimilation. Both figures also show that assimilation effectiveness is not ideal at lower altitudes, partly because background values in this range are relatively small and partly because the background field ensemble exhibits smaller sample deviations in this range. Figure 5 shows the percentage of the square root of diagonal values of background error covariance relative to ensemble sample means at 115°E, 40°N. The background error obtained from ensemble sample statistics is below 20% below 250 km, much smaller than background errors above 350 km. Smaller background values and relative deviations lead to smaller background errors, causing assimilation results to be closer to the background field and significantly reducing the improvement in deviation from observational data.

3.3 Correlation Analysis

[Figure 6: see original paper] Correlation statistics for NmF2 and hmF2 at observation profiles used in assimilation.

[Figure 7: see original paper] Correlation statistics for NmF2 and hmF2 at observation profiles not used in assimilation.

Figures 6 and 7 show scatter plots of ionospheric peak electron density (NmF2) between background field and observations before assimilation, and between analysis field and observations after assimilation. The left panels plot background field peak electron density on the x-axis against observations on the y-axis, while the right panels plot analysis field against observations. For assimilated observations, the correlation coefficient between background field and observations increases from 0.88 before assimilation to 0.98 after assimilation, with mean bias decreasing from 37.4% to -0.1% and standard deviation decreasing by approximately 60%. For unassimilated observations, the correlation coefficient improves from 0.81 to 0.94, mean bias decreases from 17.4% to 3.6%, and standard deviation decreases by approximately 20%. However, peak height assimilation results are not ideal, showing decreased mean bias but no improvement in correlation coefficient or standard deviation.

3.4 Simultaneous vs. Batch Assimilation

[Figure 8: see original paper] Comparison of electron density error statistics between simultaneous assimilation (left) and batch assimilation (right).

Simultaneously assimilating all observational data into the background field requires substantial memory. This experiment was conducted on a multi-core computer with a 1.87 GHz CPU, assimilating 3,579 observation points. Simultaneous assimilation required a maximum of approximately 8 GB memory and took 6 minutes 36 seconds. To compare simultaneous and batch assimilation, the same observational data were assimilated using batch assimilation, which required less than 2 GB memory and took 7 minutes 21 seconds. As shown in Figure 8, the comparison reveals that simultaneous and batch assimilation produce nearly identical mean bias relative to observations, but simultaneous assimilation yields relatively smaller standard deviation above 300 km altitude. This demonstrates that simultaneous assimilation offers the advantage of global optimization but requires more memory, while batch assimilation achieves good assimilation results with lower memory requirements.

---

4 Conclusions and Outlook

This paper presents the preliminary construction and experimental results of an ionospheric data assimilation model based on ensemble Kalman filter techniques. Using the ensemble Kalman filter assimilation method, COSMIC occultation electron density profiles are assimilated into the TIEGCM background model. The assimilation results demonstrate that using the ensemble Kalman filter algorithm to assimilate electron density into the background model yields good assimilation results, with standard deviation of NmF2 decreasing by approximately 60% for assimilated observations and 20% for unassimilated observations, indicating that the designed algorithm is feasible and the selected parameters are reasonable. The comparison between batch and simultaneous assimilation shows that batch assimilation requires less memory, but simultaneous assimilation produces better results with shorter computation time, making it preferable when conditions permit.

As previously mentioned, ionospheric driving parameters are crucial for ionospheric forecasting. Assimilating only electron density without optimizing ionospheric driving parameters makes reliable ionospheric forecasting difficult. The ionospheric assimilation model constructed in this paper can only be used for ionospheric nowcasting. Future work will focus on assimilation and forecasting of ionospheric driving parameters. Additionally, ionospheric forecasting assimilation involves issues such as observation data quality control, storage and computation of large matrices, and error covariance selection, requiring further algorithm optimization to improve assimilation accuracy and speed.

Acknowledgments are due to the COSMIC Data Analysis and Archive Center for providing COSMIC ionospheric occultation data and to NCAR for providing the TIEGCM model.

References

Scherliess, L., D.C. Thompson, and R.W. Schunk, Ionospheric dynamics and drivers obtained from a physics-based data assimilation model. Radio Science, 2009. 44(1).

Yue Xinan, Modeling and Data assimilation of Mid- and Low-Latitude Ionosphere. [D]. 2008, Wuhan Institute of Physics and Mathematics, Graduate University of Chinese Academy of Sciences.

Schunk, R.W., et al., Global assimilation of ionospheric measurements (GAIM). Radio Science, 2004. 39(1).

Scherliess, L., et al., Development of a physics-based reduced state Kalman filter for the ionosphere. Radio Science, 2004. 39(1).

Scherliess, L., et al., Utah State University Global Assimilation of Ionospheric Measurements Gauss-Markov Kalman filter model of the ionosphere: Model description and validation. Journal of Geophysical Research: Space Physics (1978-2012), 2006. 111(A11).

Matsuo, T., I.T. Lee, and J.L. Anderson, Thermospheric mass density specification using an ensemble Kalman filter. Journal of Geophysical Research: Space Physics, 2013. 118(3).

Lee, I., et al., Assimilation of FORMOSAT-3/COSMIC electron density profiles into a coupled thermosphere/ionosphere model using ensemble Kalman filtering. Journal of Geophysical Research: Space Physics (1978–2012), 2012. 117(A10).

Evensen, G., The ensemble Kalman filter for combined state and parameter estimation. Control Systems, IEEE, 2009. 29(3): p. 83-104.

Yue, X., et al., Error analysis of Abel retrieved electron density profiles from radio occultation measurements. Annales Geophysicae, 2010. 28(1): p. 217-222.

Bust, G., T. Garner, and T. Gaussiran, Ionospheric Data Assimilation Three-Dimensional (IDA3D): A global, multisensor, electron density specification algorithm. Journal of Geophysical Research: Space Physics (1978–2012), 2004. 109(A11).

Yue, X., et al., Data assimilation of incoherent scatter radar observation into a one-dimensional midlatitude ionospheric model by applying ensemble Kalman filter. Radio Science, 2007. 42(6).

Yue X A, Wan W X, Liu L B, et al. Development of an ionospheric numerical assimilation nowcast and forecast system based on Gauss-Markov Kalman filter —An observation system simulation experiment taking example for China and its surrounding area. Chinese J. Geophys. (in Chinese), 2010, 53(4): 787-795.

Hmaill, T.M., Ensemble-Based Data Assimilation. Workshop on Predictability ECMWF, 2002.

Note: Figure translations are in progress. See original paper for figures.