1 Analysises of different propagation models for the estimation

of the topside ionosphere and plasmasphere with an Ensemble Kalman Filter

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9 Abstract.

10 The accuracy and availability of satellite-based applications like GNSS positioning and remote sensing crucially

11 depends on the knowledge of the ionospheric electron density distribution. The tomography of the ionosphere is

12 one of the major tools to provide link specific ionospheric corrections as well as to study and monitor physical

13 processes in the ionosphere and plasmasphere. In this work, we apply an Ensemble Kalman Filter (EnKF) approach

- 14 for the 4D electron density reconstruction of the topside ionosphere and plasmasphere with the focus on the
- 15 investigation of different propagation models and compare them with the iterative reconstruction technique
- 16 SMART+. The STEC measurements of eleven LEO satellites are assimilated into the reconstructions. We conduct
- 17 a case study on a global grid with altitudes between 430 and 20200 km, for two periods of the year 2015 covering
- 18 quiet to perturbed ionospheric conditions. Particularly, the performance of the methods to estimate independent
- 19 STEC and electron density measurements from the three Swarm satellites is analysed. The results indicate that the
- 20 methods EnKF with Exponential decay as the propagation model and SMART+ perform best, providing in
- 21 summary the lowest residuals.

22 1 Introduction

- 23 The ionosphere is the <u>charged upper</u> part of the <u>upper</u> atmosphere extending from about 50 1000 km and going 24 over in the plasmasphere. The characteristic property of the ionosphere is that it contains sufficient free electrons 25 to affect the <u>radio waves</u> propagation of trans-ionospheric radio signals, as from telecommunication, navigation or
- 26 remote sensing satellites, by refraction, diffraction and scattering.
- 27 Therefore, the knowledge of the three-dimensional electron density distribution and <u>itstheir</u> dynamics are of 28 practical importance. Around 50% of the signal delays or range errors of L-band signals used in GNSS originate 29 from altitudes above the ionospheric F2 layer, <u>consistingwhich consist</u> of topside ionosphere going over into 30 thande plasmasphere (cf. Klimenko et al., 2015; Chen and Yao, 2015). So far, especially the topside ionosphere
- 31 and plasmasphere is not well described.
- 32 The choice of the ionospheric correction model has an essential impact on the accuracy of the estimated
- 33 ionospheric delay and its uncertaint<u>yies</u>. A widely used approach for ionospheric modelling is the single-layer
- 34 model, whereby the ionosphere is projected onto a two-dimensional (2D) spherical layer, typically located between
- 35 350 and 450 km. However, usually 2D models are not accurate enough to support high accuracy navigation and
- 36 positioning techniques in real time (cf. e.g. Odijk 2002; Banville 2014). Additionally, they do not provide the
- 37 possibility to look insight the complex coupling processes between magnetosphere, plasmasphere and ionosphere.
- 38 More accurate and precise positioning is achievable by considering the ionosphere as 3D medium. There are

39 several activities in the ionosphere community aiming to describe the me<u>andian</u> ionospheric behavior by the

40 development of 3D electron density models based on long-term historical data. Two widely used models are the

41 International Reference Ionosphere model (IRI, cf. Bilitza et al., 2011) and the NeQuick model (cf. Nava et al.,

42 2008).

43 Since those models represent a median-mean behavior, it is essential to update them by the assimilation of actual 44 ionospheric measurements. There is a variety of approaches developed and validated for the ionospheric 45 reconstruction by the combination of actual observations with an empirical or a physical background model. 46 Hernandez-Pajares et al. (1999) present one of the first GNSS-based data-driven tomographic models, which 47 considers the ionosphere as a grid of three-dimensional voxels and the electron density within each voxel is 48 computed as a random walk time series. The voxel-based discretisation of the ionosphere is further used for 49 instance in Heise et al., 2002; Wen et al., 2007; Gerzen and Minkwitz, 2016; Gerzen et al., 2017; Wen et al., 50 2020. These authors reconstruct the 3D ionosphere by algebraic iterative methods. An alternative is to estimate the 51 electron density as a linear combination of smooth and continuous basis functions, like e.g. spherical harmonics 52 (SPH) (Schaer 1999), B-splines (Schmidt et al., 2008; Zeilhofer, 2008; Zeilhofer et al., 2009: 40; Olivares-Pulido 53 et al., 2019), B-splines and trigonometric B-splines (Schmidt et al. 2015), B-splines and Chapman functions (Liang

et al., 2015 and 2016), and empirical orthogonal functions and spherical harmonics (Howe et al., 1998).

Besides the algebraic methods, also techniques taking benefit of information on spatial and temporal covariance
information, such as Optimal Interpolation, Kalman Filter, three- and four-dimensional variational techniques and

57 Kriging, are applied to update the modelled electron density distributions; (cf. Howe et al., 1998; Angling et al.,

58 2008; Minkwitz et al., 2015 and 2016; Nikoukar et al., 2015; Olivares-Pulido et al., 2019).

Moreover, there are approaches based on physical models, which combine the estimation of the electron density
with physical related variables such as neutral winds or the oxygen/nitrogen ratio (cf. Wang, et al. 2004; Scherliess
et al., 2009; Lee et al., 2012; Lomidze et al., 2015; Schunk, et al., 2004 and 2016; Elvidge and Angling, 2019).

In general, the majority of data, available for the reconstruction of the ionosphere and plasmasphere, are Slant
Total Electron Content (STEC) measurements, i.e. the integral of the electron density along the line of sight
between the GNSS satellite and receiver. Often, STEC measurements provide limited vertical information and

hence the modelling of the vertical the electron density distribution is hampered (<u>cf. e.g.</u> Dettmering, 2003).

66 The estimation of the topside ionosphere and plasmasphere poses a particular difficulty since direct electron67 density measurements are rare and since low plasma densities at these high altitudes contribute only marginally to

the STEC measurements. Especially, ground-based STEC measurements are dominated by electron densities

69 within and below the characteristic F2 layer peak. Consequently, information about the plasmasphere can be

70 hardlyis difficult to extracted from ground-based STEC measurements, (cf. e.g. Spencer and Mitchell, 2011). Thus,

in the presented work, we concentrate on the modeling of the topside part of the ionosphere and plasmasphere and

72 utilize only the space-based STEC measurements.

73 In this paper, we introduce an Ensemble Kalman Filter to estimate the topside ionosphere and plasmasphere based

74 on space-based STEC measurements. The propagation of the analyszed state vector to the next time step within a

75 Kalman Filter is a key challengetricky point.- The majority of the approaches, working with EnKF variants, uses

76 physic-based models for the propagation step (cf. e.g. Elvidge and Angling 2019; Codrescu et al., 2018; Lee et al.,

77 2012). In our work, we investigate the question how the propagation step can be realized, if a physical model is

78 not available or if the usage of a physical model is rejected as computationally-time consuming. We discretize the

- ionosphere and the plasmasphere below the GNSS orbit height by 3D voxels, initialize them with electron densities

- 80 calculated by the NeQuick model and update them with respect to the data. We present different methods how to
- perform the propagation step and assess their suitability for the estimation of electron density. For this purpose, a
- 82 case study over quiet and perturbed ionospheric conditions in 2015 is conducted, investigating the capability of
- 83 the estimateions to reproduce assimilated STEC as well as to reconstruct independent STEC and electron density
- 84 measurements.

We organize the paper as follows: Section 2 describes the EnKF with the different propagation methods and the generation of the initial ensembles by the NeQuick model. Section 3 outlines the validation scenario with the applied data sets<u>__and_S</u>ection 4 presents the obtained results. Finally, we conclude our work in <u>Section 5</u> and

88 provide an outlook on the next steps.

89 2 Estimation of the topside ionosphere and plasmasphere by EnKF

90 2.1 Formulation of the underlying inverse problem

91 The information about the slant total electron content (STEC), along the satellite-to-receiver ray path s can be
92 obtained from multi-frequency GNSS measurements. In detail, STEC is a function of the electron density *Ne*93 along the ray path s, given by

$$STEC_s = \int Ne(h,\lambda,\varphi)ds,$$
 (1)

- 94 where $Ne(h, \lambda, \varphi)$ is the unknown function describing the electron density values depending on altitude h, 95 geographic longitude λ and latitude φ .
- 96 The discretization of the ionosphere by a 3D grid and the assumption of a constant electron density function within 97 a fixed voxel allow-us the transformation of Eq. (1)(1) into a linear system of equations

$$STEC_s \approx \sum_{i=1}^{K} Ne_i \cdot h_{si} \Rightarrow y = Hx + r, \tag{2}$$

where y is the $a-(m \times 1)$ vector of the STEC measurements, x is the vector of unknown electron densities with $x_i = Ne_i$ equals the electron density in the voxel i, h_{si} is the length of the ray path s in the voxel i and r is the vector of measurement errors assumed to be Gaussian distributed with $r \sim N(0, R)$ with expectation 0 and covariance matrix R.

102 2.2 Background model

As regularisation of the inverse problem in Eq. (2)(2), a background model often provides the initial guess of the state vector *x*. In this study, we apply the NeQuick model version 2.0.2. The NeQuick model was developed at the International Centre for Theoretical Physics (ICTP) in Trieste/Italy and at the University of Graz/Austria (cf. Hochegger et al., -(2000); Radicella and Leitinger, -(2001); Nava et al., -(2008)). <u>TWe use the daily solar flux</u> index F10.7 is used; to drive the NeQuick model.

108 2.3 Analysis step of the EnKF

We apply an EnKF to solve the inverse problem defined in Section 2.1. Evensen (1994) introduces the EnKF as an alternative to the standard Kalman Filter (KF) in order to cope with the non-linear propagation dynamics and the large dimension of the state vector and its covariance matrix. In an EnKF, a collection of realisations, called ensembles, represent the state vector x and its distribution.

- 113 Let $X^f = [x_1^f, ..., x_{NK}^f]$ be a $(K \times N)$ matrix whose columns are the ensemble members, ideally following the a
- priori distribution of the state vector x. Further, the observations collected in y are treated as random variables. Therefore, we define an $(m \times N)$ - ensemble of observations $Y = [y_1, y_2, ..., y_N] \leftarrow$ with $y_i = y + \epsilon_i$ and a random vector ϵ_i from the normal distribution N(0, R).
- 117 We define the ensemble covariance matrix around the ensemble mean $E(X^f) = \frac{1}{N} \sum_{j=1}^{N} x_j^f$ as follows:

$$P^{f} = \frac{1}{N-1} \sum_{j=1}^{N} \left\{ \left(x_{j}^{f} - E(X^{f}) \right) \cdot \left(x_{j}^{f} - E(X^{f}) \right)^{T} \right\}.$$
(3)

118 In the analysis step of the EnKF, the a priori knowledge on the state vector x and its covariance matrix is updated 119 by

$$X^{a} = X^{f} + P^{f} H^{T} (R + HP^{f} H^{T})^{-1} \cdot (Y - HX^{f}),$$
⁽⁴⁾

120 where the matrix X^a represents the a posteriori ensembles and hence the a posteriori state vector.

For the propagation of the analysed solution to the next time step, we test different propagation models described in Section 2.4. In order to generate the initial ensembles $X^f(t_0)$ we use the NeQuick model and describe the procedure in Section 2.5. Keeping in mind that we have to deal with an extremely large-huge state vector (details are presented in Section 3.1), the important big advantage of the EnKF, for the present study, is that there is no need for explicitly calculation of the ensemble covariance matrix (cf. Eq. (3)(3)). Instead, to perform the analysis step in Eq. (4)(4) we follow the implementation suggested by Evensen (2003).

127 2.4 Considered models for the propagation step of the EnKF

- 128 In this section, we introduce the different models-investigated to propagate the analysed solution to the next time 129 step. With all of them, we propagate the ensembles 20 minutes in time. <u>Generally, t</u>These propagation models can 130 be generally described as $X^{f}(t_{n+1}) = F(X^{a}(t_{n})) + W_{F}(t_{n+1}) + \Omega_{F}(t_{n+1})$. In the following subsections,
- 131 <u>wWe outline possible choices</u> applied different approaches of the to model F, the systematic error W_F and the
- 132 process noise Ω_F and present in this paper a selection of the most promising variants of them.
- 133 Note: Beyond the presented methods, in addition we had tested a propagation model based on "persistence", i.e. 134 $X^{f}(t_{n+1}) = X^{a}(t_{n}) + W_{persisF}(t_{n+1}) + \Omega_{persis}(t_{n+1})$. Already after a time period of about 24 hours, this method
- 135 <u>had shown unreasonable effects in the reconstructions, like a completely misplaced equatorial crest region.</u>
- 136

137 2.4.1 Method 1: Rotation

138 The method Rotation assumes that in <u>geo</u>magnetic coordinates, the ionosphere remains invariant in space while 139 Earth rotates below it (cf. Angling and Cannon, 2004). Thus, we propagate the analysed ensemble $X^a(t_n)$ from 140 time t_n to the next time step t_{n+1} by:

$$X^{f}(t_{n+1}) = Rot(X^{a}(t_{n})) + W_{rot}(t_{n+1}).$$
⁽⁵⁾

141 <u>**TIn detail, to calculate** $Rot(X^a(t_n))$ the geomagnetic longitude is changed corresponding to the evolution time 142 $\Delta t = t_{n+1} - t_n$, i.e. 5 degree of longitude per 20 minutes. W_{rot} denotes the systematic error introduced by 143 approximation of the true propagation of X^f by a simple rotation. We tested here the following estimation of W_{rot} :</u>

$$W_{rot}(t_{n+1}) = ratio_{rot}(t_{n+1}) \cdot E\left(Rot(X^{a}(t_{n}))\right) \cdot \epsilon_{1 \times N} \text{ withand } ratio_{rot}(t_{n+1}) = \frac{\left(x^{b}(t_{n+1}) - Rot(x^{b}(t_{n}))\right)}{3 \cdot Rot(x^{b}(t_{n}))}, \quad (6)$$

$$ratio_{rot}(t_{n+1}) = \frac{\left(x^b(t_{n+1}) - Rot(x^b(t_n))\right)}{3 \cdot Rot(x^b(t_n))},\tag{76}$$

167 where x^b is the electron density vector calculated by the NeQuick model and $\epsilon_{1\times N}$ is an $(1 \times N)^{1-by-N}$ matrix of 168 ones. The division in the second equation is an element-wise-one. The ratio $ratio_{rot}(t_{n+1})$ in Eq. (7)(7) represents 169 the relative error introduced by the application of $Rot(x^b(t_n))$ instead of $x^b(t_{n+1})$. In this way, we obtain in Eq. 169 (6) an approximation of the mean error introduced by approximation of the true state at time t_{n+1} by the a-rotation 170 of the true state at time t_n . The factor $\frac{1}{3}$ has been chosen empirically as the result₃ of an internal validation not 172 presented within this paper.

173 2.4.2 Method 2: Exponential decay

Here we assume the electron density differences between the voxels of the analysis and the background model to
be a first order Gauss-Markov sequence. These differences are propagated in time by an exponential decay function
(cf. Nikoukar et al. 2015, Bust and Mitchell, 2008; Gerzen et al., 2015)

$$X^{f}(t_{n+1}) = X^{b}(t_{n+1}) \cdot \epsilon_{1 \times N} + f(t_{n+1}) \cdot [X^{a}(t_{n}) - X^{b}(t_{n})],$$
(87)

177 where $X^{b}(t)$ is the ensemble of electron density vectors calculated by the NeQuick model for the time *t* as 178 described in <u>Section 2.5;</u> $f(t_{n+1}) = \exp\left(-\frac{\Delta t}{\tau}\right)$; $\Delta t = t_{n+1} - t_n$; τ denotes the temporal correlation parameter 179 chosen here as 3 hours.

180 Note: Similar to the method described here, we tested also the application of $Rot([X^a(t_n) - X^b(t_n)])$ instead of 181 $[X^a(t_n) - X^b(t_n)]$ in Eq. (8)(7). The results were similar and are therefore not presented here.

182 2.4.3 Method 3: Rotation with exponential decay

For the As third method, we define the propagation model as a combination of the propagation models described
 in the previous subsections, in particular

$$X^{f}(t_{n+1}) = x^{b}(t_{n+1}) \cdot \epsilon_{1 \times N} + f(t_{n+1}) \cdot Rot([X^{a}(t_{n}) - x^{b}(t_{n}) \cdot \epsilon_{1 \times N}]) + W(t_{n+1}) + \sqrt{\frac{\Delta t}{20}} \cdot \Omega_{exp}(t_{n+1}).$$
(98)

185 The systematic error *W* is estimated as

$$W(t_{n+1}) = f(t_{n+1}) \cdot \frac{8}{10} \cdot W_{rot}(t_{n+1}).$$
(109)

186 Thereby f and W_{rot} are defined as in the two previous sections bevor. The factor $\frac{8}{10}$ thereby is again chosen 187 empirically. The process noise Ω_{exp} is assumed to be white with $\Omega_{exp}(t_{n+1}) = f(t_{n+1}) \cdot \Omega_{rot}(t_{n+1}) +$ 188 $(1 - f(t_{n+1})) \cdot Q_{exp}(t_{n+1})$. Here the matrix Ω_{rot} consists of random realizations of the distribution $N(0, \Sigma^{rot})$ 189 with Formatie

$$\Sigma_{ii}^{rot}(t_{n+1}) = \left(ratio_i \cdot \left\{ E\left(Rot(X^a(t_n))\right) \right\}_i \right)^2, \qquad (\underline{1140})$$

where $ratio_i$ increases continuously depending on the altitude of the voxel *i* from $\frac{0.5}{100}$ for lower altitudes to $\frac{1}{100}$ for the higher altitudes (chosen empirically); $E\left(Rot(X^a(t_n))\right)$ denotes the ensemble mean vector. The equations (9)(8) and (11)(10) can be interpreted as follows: Effor the chosen time step of 20 minutes, the standard deviation of the time model error regarding the voxel *i* is equal to $\sqrt{\sum_{ii}^{rot}(t_{n+1})} = ratio_i \cdot \left\{ E\left(Rot(X^a(t_n))\right) \right\}_i$, varying between 0.5% and 1% of the corresponding analyszed electron density in the voxel *i*. In details, we generate at each time step a new vector $\rho_i \sim N(0,1)$ with dim $(\rho_i) = 100 \times 1$ and calculate to calculate the *i*-th row ω_i^{rot} of Ω_{rot} by Eq. Fehler! Verweisquelle konnte nicht gefunden werden..

$$\omega_i^{rot}(t_{n+1}) = \sqrt{\Sigma_{ii}(\Omega_{rot}(t_{n+1}))} \cdot \rho_i(t_{n+1})^T.$$
(121211)

228

The matrix $Q_{exp}(t_{n+1})$ consists of random realizations (different for each time step) consistent with the a priori covariance matrix *L* of the errors of the background $x^b(t_{n+1})$ (cf. Howe and Runciman, 1998). In details: The a priori covariance is assumed to be diagonal and L_{ii} equals the square of 1% of the corresponding background model value. Then the *i*-th row of Q_{exp} is calculated by Eq. (13)(12):

$$q_i(t_{n+1}) = \sqrt{L_{ii}(t_{n+1})} \cdot \rho_i(t_{n+1})^T.$$
(1342)

233 2.5 Generation of the ensembles

In order to generate the ensembles we vary the F10.7 input parameter of the NeQuick model (cf. Section 2.2). First, we analysed the sensitivity of the NeQuick model on F10.7. Based on the results, we calculate a vector **F10.7**(*t*) of the solar radio flux index with dim(*F*10.7(*t*)) = 100 × 1 and *F*10.7(*t*)~N(F10.7(*t*), $\frac{3}{100}$ · F10.7(*t*)) at time *t*. The vector *F*10.7 serves as input for the NeQuick model to calculate the 100 ensembles of *X^b* during the considered period and the initial guess of the electron densities *X^f*(*t*₀). An example on the variation of the generated ensembles is provided by <u>Figure 1</u>Figure 1. Particularly, we show

in this figure the distribution of the differences between the ensemble of electron densities $X^b(t)$ and the NeQuick model values for DOYs 041 and 076. The residuals are depicted for a selected altitude and chosen UT times, presented through different colors (cf. subfigure history). In addition, the mean, the standard deviation (STD) and the root mean square (RMS) of the residuals are presented in the subplots.

244 2.6 Provision of a benchmark by SMART+

- 245 <u>In order to provide a benchmark for the described methods, we apply SMART+ as an additional reconstruction</u>
 246 <u>technique.</u>
- 247 <u>SMART+ is a combination of an iterative simultaneous multiplicative column normalized method SMART (cf.</u>
- 248 Gerzen and Minkwitz, 2016) and a 3D successive correction method (3D SCM) (cf. e.g. Kalnay, 2011; Gerzen
- and Minkwitz, 2016). -As fFirst step, SMART distributes the STEC measurements among the electron densities
- 250 in the ray-path intersected voxels. For a fixed-voxel-*i*, the multiplicative innovation is calculated as a weighted
- 251 mean of the ratios between the actual measurements and the currently expected measurements. The weights are

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- given by the length of the ray path corresponding to the measurement in the voxel *i* divided by the sum of lengths
- 253 of all rays crossing the voxel- *i*. Consequently, only voxels intersected by at least one measurement-ray path, are
- 254 innovated during the SMART procedure. Thereafter, assuming non-zero correlations between the ray path
- 255 intersected voxels and those not intersected by any STEC-, an extrapolation is done from intersected to not
- 256 intersected voxels. For this purpose, one iteration of the 3D SCM is applied. For more details we refer to- Gerzen
- and Minkwitz (2016) and Gerzen et al. (2017).
- 258 For SMART+ the number of iterations at each time step is set to 25 and the correlation coefficients are chosen as
- 259 <u>described in Gerzen and Minkwitz (2016). For each time step, SMART+ reconstructs the electron densities based</u>
- on the background model (here NeQuick) and the currently available measurements. In other words, there is no
- 261 propagation of the estimated electron densities from a time step t_n to the time step t_{n+1} .

262 3 Validation scenario

Within this study, the EnKF with the different propagation methods is applied and validated for the tomography of the topside ionosphere and plasmasphere. <u>TParticularly, two</u> periods with quiet (DOY 041-059, 2015) and perturbed (DOY 074-079, 2015) ionospheric conditions are analysed. In this scope, we investigate the ability to reproduce assimilated STEC as well as to estimate independent STEC measurements and in-situ electron density measurements of the Swarm Langmuir Probes (LP).

In addition, we apply the tomography approach SMART+ (<u>cf. Section 2.6</u>Gerzen and Minkwitz, 2016 and Gerzen
 et al., 2017) to provide a benchmark. For SMART+ the number of iterations at each time step is set to 25 and the
 correlation coefficients are chosen as described in Gerzen and Minkwitz (2016).

271 3.1 Reconstruction area

We estimate the electron density over the entire globe with a spatial resolution of 2.5 degrees in <u>geodetic</u> latitude and longitude. Altitudes between 430 km and 20 200 km are reconstructed where the resolution equals 30 km for altitudes from 430 km to 1000 km and decreases exponentially with increasing altitude for altitudes above 1000 km, i.e. in total 42 altitudes. Consequently, the number of unknowns is K = 217728. The temporal resolution Δt is set to 20 minutes.

277 3.2 Ionospheric conditions in the considered periods

We use the solar radio flux F10.7, the global planetary 3h index Kp and the geomagnetic disturbance storm time
(DST) index to characterize the ionospheric conditions during the periods of DOY 041-059 and DOY 074-079
2015. In the February period (DOY 041-059, 2015) the ionosphere is evaluated as quiet with F10.7 between 108
and 137 sfu, a Kp index below 6 (on two days between 4 and 6, during the rest of the period below 4) and DST
values between 20 and -60 nT. The 17-th of March (DOY 076) 2015 is known as the St. Patrick's Day storm. The
F10.7 value equals ~116 sfu on DOY 075 and ~113 sfu on DOY076, the Kp index is below 5 on DOY 075 and
increases to 8 on DOY 076; DST drops down to -200nT on DOY 076.

285 3.3 Data

286 3.3.1 STEC measurements

- 287 As input for the tomography approaches and for the validation, we use space-based calibrated STEC measurements
- of the following LEO satellite missions: COSMIC satellites, Swarm, -satellites, TerraSAR-X, X, MetOpA and
- 289 MetOpB, and, GRACE-LEO satellites. Please note that in 2015, the orbit height of the COSMIC and MetOp
- satellites is ~800 km, the orbit height of the Swarm B and TerraSAR-X satellites is ~500 km and the one of the
- Swarm C satellite ~460 km. The STEC measurements of Swarm A and GRACE are used-only for the validation
- 292 <u>only. The Swarm A satellite flew side by side on site with the Swarm C satellite at around 460 km height. The</u>
- 293 <u>height of the GRACE orbit was around 430 km. All satellites flew at almost polar orbits.</u> More information about
- 294 <u>the LEO satellites may be found on the following webpages:</u>
- 295 <u>COSMIC: https://www.nasa.gov/directorates/heo/scan/services/missions/earth/COSMIC.html)</u>,
- 296 <u>Swarm: (https://www.esa.int/Applications/Observing the Earth/Swarm),</u>
- 297 <u>TerraSAR-X: (https://earth.esa.int/web/eoportal/satellite-missions/t/terrasar-x),</u>
- 298 MetOpA and MetOpB: (https://directory.eoportal.org/web/eoportal/satellite-missions/m/metop),
- 299 <u>GRACE: (https://www.nasa.gov/mission_pages/Grace/index.html).</u>
- 300 The STEC measurements of the Swarm satellites are acquired from https://swarm-diss.eo.esa.int/ and the STEC 301 of measurements the other satellite missions are downloaded from http://cdaac-302 www.cosmic.ucar.edu/cdaac/tar/rest.html. Both data providers supply also information on the accuracy of the 303 STEC data. We utilize this information to fill the covariance matrix R of the measurement errors. The collected 304 STEC data is checked for plausibilityfiltered before the assimilation-.

305 3.3.2 In-situ electron density measurements from the Swarm Langmuir Probes

- The LPs on board the Swarm satellites provide in-situ electron density measurements with a time resolution of 2
 Hz. For the present study, the LP in-situ data are acquired from https://swarm-diss.eo.esa.int/. In addition, fFurther,
 information on the pre-processing of the LP data is made available.
- 309 Lomidze et. al (2018) assess the accuracy and reliability of the LP data (December 2013 to June 2016) by nearly
- 310 coincident measurements from low- and middle-latitude incoherent scatter radars, low-latitude ionosondes, and
- 311 COSMIC satellites, which cover all latitudes. The comparison results for each Swarm satellite are consistent across
- these different measurement techniques. The results show that the Swarm LPs underestimate the electron density
- systematically by about 10%.

314 4 Results

- In this section, the different methods are presented with the following color code: blue for the method Rotation,
- green for the method Exponential decay, light blue for the method Rotation with exponential decay, magenta for
- 317 NeQuick and red for SMART+. The legends in the figures are the following: "Rot" for the method Rotation, "Exp"
- 318 for the method Exponential decay, "Rot and Exp" for the method Rotation with exponential decay.

319 4.1 Reconstructed electron densities

332

320 At the end of each EnKF analysis step, we have, for each of the considered methods, 100 ensembles representing 321 the electron density values within the voxels. The EnKF reconstructed electron densities are then calculated as the 322 ensemble mean. The top subplots of Figure 2Figure 2 present the electron densities at DOY 076, 19:00 UT, reconstructed by the method Rotation with exponential decay, i.e. $\underline{-(i.e.}E(X_{Rot and Exp}^{a}(t_{n}))$, for t_{n} corresponding 323 324 to DOY 076, at 19:00 UT). The left hand sideupper left corner subplot shows horizontal layers of the topside 325 ionosphere at different heights between 490 and 827 km. The -right hand side subplot in the upper right corner t 326 illustrateshows the plasmasphere for altitudes between 827 and 2400 km at chosen-selected longitudes. The bottom 327 line subplots show the vertical-VTEC maps deduced from the 3D electron density in the considered altitude range 328 between 430 and 20200 km-for the same time stamp, where the left hand side subplot represents show the 329 reconstructed values and the right hand side VTEC is deduced calculated from the NeQuick model-calculated 330 electron density. It is observed that the reconstructed VTEC values are slightly a bit higher than the ones 331 of the NeQuick modelones.

333 Figure 3 Figure 3 displays the electron density layers reconstructed by the method Rotation-reconstructed electron 334 density layers, -(i.e. $E(X_{Rot}^a(t_n))$, for t_n equal corresponding to DOY 076, at 19:00 UT.) at different Again, 335 reconstructed electron densities at heights between 490 and 827 km (left) and the corresponding Vvertical-TEC 336 map_deduced from the reconstructed 3D electron density in the altitude range between 430 and 20200 km (right) 337 are depicted. All reconstructed values seem to be plausible, showing as expected the crest region, low electron 338 densities in the Polar regions, etc. The method Rotation delivers much higher values than the NeQuick model, cf. 339 Figure 2Figure 2. In Figure 4, we take a closer look at the differences between the modelled and reconstructed 340 electron densities. All reconstructed values seems to be plausible, showing as expected the crest region, low 341 electron densities in the Polar regions, etc.

342 In the following, we discuss Figure 4-Figure 4 - Figure 7Figure 7, in order to understand the deviations between 343 the reconstructions produced byof the different methods. On Figure 4Figure 43 the differences <u>between the reconstructed and the modelled electron densities, (i.e.</u> $E(X^a(t_n)) - x^b(t_n), \frac{1}{2}$ and modeled (i.e. 344 $x^{b}(t_{n})$ electron densities are shown for all -methods: EnKF with Rotation with exponential decay-as forecast 345 346 function,: EnKF with Rotation,: EnKF with Exponential decay and: SMART+ (from top left subfigure to bottom 347 right subfigure) on DOY 076 at 19:00 UT. In addition, -Figure 5Figure 54 expresses these differences in percent. 348 Please note the different ranges of the colorbars for the subfigures. Figure 6 illustrating es the orbits of the LEO 349 satellites for the STEC measurements used for the reconstructions on DOY 076, at 19:00 UT (left) and the 350 corresponding ground-track (right). The highest differences are observed for the mMethods Rotation and 351 Exponential decay, whereas the method Rotation with exponential decay yields, the smallest differences-. 352 Furthermore, as expected, the EnKF approaches provide smooth and coherent patterns of differences in the 353 ionization. Contrary, the complementary approach of SMART+ has rather small patterns in areas where 354 measurements are available and falls back to the background model in areas without measurements in the 355 surrounding. In this context, the correlation lengths between the electron densities are of importance. These 356 correlation lengths are set empirically in SMART+, whereas EnKF establishes them automatically, i.e. without 357 setting or estimating them explicitly as for instance in SMART+ or Kriging approaches. For a comprehensive 358 evaluation of Future analyses are necessary which evaluate the quality of the different reconstructions in the 390 context of the used correlation lengths, future analyses with further validation data and in dependence on the 391 coincidences between the measurement geometry and the geometry of the validation data set are necessary. Taking into account the differences in -Figure 5, for instance around 120°E, and the measurement geometry in 392 393 Figure 6Figure 6, it is evident that the estimates of the EnKF are not only based on the current measurements but 394 also on a priori information obtained from assimilations before DOY 076, -2015, 19:00 UT. This is of course not 395 the case for SMART+. 396 In order to supplement the understanding on the differencesf -between the different propagation methods, Figure <u>7 presents the differences $E\left(X_{method}^{f}(t_{n+1})\right) - E\left(X_{method}^{a}(t_{n})\right)$ on the left column subfigures; and the</u> 397 differences 398 percentageal $100 \cdot$ $\left[E\left(X_{method}^{f}(t_{n+1})\right) - E\left(X_{method}^{a}(t_{n})\right) \right] / \frac{1}{2} \cdot \left[E\left(X_{method}^{f}(t_{n+1})\right) + E\left(X_{method}^{a}(t_{n})\right) \right]$ in the right column, for t_{n} 399 400 corresponding to DOY 076, at 19:00 UT. Particularly, for the methods (from top to bottom): Rotation with exponential decay, Rotation and, Exponential decay are presented. The differences for the methods Rotation and 401 402 Rotation with exponential decay clearly indicate the rotation of the crest region (cf. also **Figure 3**). The method Rotation with exponential decay works less rigorously in the rotation than the method Rotation since it is 403 anchored by the background model and the rotation of the differences $X^{a}(t_{n}) - x^{b}(t_{n})$ is damped by the 404 405 exponential decay function, see Eq. (9(9)). Contrary to these two methods, the method Exponential decay tries to <u>propagate the difference</u> $X^{a}(t_{n}) - X \mathbf{x}^{b}(t_{n})$ to the next time step and adds them to the background $X^{b}(t_{n+1})$. 406

407 <u>Hence, we observe in the lower left corner subplot of Figure 7Figure 7</u> a similar pattern as in the corresponding

408 <u>lower left corner subplot of Figure 4Figure 4</u>.

409 Concluding, the different behaviour of the propagation methods in combination with the sparse measurement

- geometry might serve as an explanation for the substantial differences observed in the VTEC maps shown in
- 411 Figure 2Figure 2 and Figure 3Figure 3.

412 4.2 Plausibility check by comparison with assimilated STEC

In this <u>Sectionehapter</u>, we check the ability of the methods to reproduce the assimilated STEC measurements. For that purpose, we calculate STEC along a ray path *j*, for all ray path geometries, using the estimated 3D electron densities, denoted as $STEC_j^{est}$, and compare them with the measured STEC, $STEC_j^{meas}$, used for the reconstruction. Then the mean deviation $\Delta STEC$ between the measurements $STEC_j^{meas}$ and the estimate $STEC_j^{est}$ is calculated for each of the considered methods according to

$$\Delta STEC(t_n) = \frac{1}{m} \sum_{j=1}^m (|STEC_j^{meas}(t_n) - STEC_j^{est}(t_n)|), \qquad (\underline{1413})$$

418 where m = number of assimilated measurements. $\Delta STEC$ is calculated at each epoch t_n . In terms of the notation 419 used for the Eqs. (1)(1) - (4)(4), we can reformulate the above formula for the mean deviation as

$$\Delta STEC(t_n) = \frac{1}{m} \sum_{j=1}^m \left(|y_j(t_n) - E(X_a(t_n))^T \cdot H_j| \right), \text{ with } H_j = j \text{-th row of } H.$$
(1514)

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Further, we consider the **RMS** of the deviations, in detail

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$$RMS(t_n) = \sqrt{\frac{1}{m} \sum_{j=1}^{m} (|STEC_j^{meas}(t_n) - STEC_j^{est}(t_n)|)^2}.$$
 (1615)

457 To calculate $\Delta STEC$ and *RMS*, the same measurements are used as for the reconstruction. In this sense, the results 458 presented in <u>Figure 8Figure 4</u> - <u>Figure 12Figure 8</u> can serves as a plausibility check, testing the ability of the 459 methods to reproduce the assimilated TEC.

Figure 8Figure 4 depicts the distribution of the residuals, left subfigure for the quiet period, right subfigure for
the perturbed period. The corresponding residual median, standard deviation (STD) and root mean square (RMS)
values are also presented in the figure. It is worth to mention here that during the quiet period, the measured STEC
is below 150 TECU. For all DOYs of the perturbed period, except DOY 076, the measured STEC is below ~130
TECU. On DOY 076, the STEC values rise up to 370 TECU.

465 The NeQuick model seems to underestimate the measured topside ionosphere and plasmasphere STEC during both 466 periods. During both periods, SMART+ seems to perform best, followed by the method Rotation. However, the 467 last oneRotation produces higher STD and RMS values. Compared to the NeQuick residuals, SMART+ is able to 468 reduce the median of the residuals by up to 86% during the perturbed and up to 79% during the quiet period. The 469 RMS is reduced by up to 48% and the STD by up to 41%. Rotation reduces the NeQuick median by up to 83%, 470 the RMS by up to 27%, the STD value is almost on the same level as for NeQuick. The method Exponential decay 471 is able to decrease the median of the NeQuick residuals by up to 54%, the RMS by up to 25%, and the STD values 472 by up to 13%. The method Rotation with exponential decay performs similar to the NeQuick model. The latter 473 could indicate that the parameters chosen for the error terms and weighting in Eq. (9) could still be improved, 474 although an extensive validation of these parameters was performed prior to the analyses presented in this paper 475 and the best configuration was selected.

476

Interestingly, the median values are higher during the quiet period, while during the perturbed period the RMS and
the STD values are on the same level compared between perturbed and quiet periods. The reason therefore is
probably that the assimilated STEC values have in average lower magnitude during the days in the perturbed
period, compared to those during the quiet period (which explains the lower median), except the storm DOY 076,
while on DOY 076 they are significantly higher (which explains the <u>comparable</u> STD and RMS).

482 Figure 9Figure 5 and Figure 10Figure 6 plot $\Delta STEC$ values versus time for the selected periods. Noticeable is 483 the increase of $\Delta STEC$ during the storm on DOY 76. On the rest of the period, $\Delta STEC$ is below eight TECU. 484 During both periods, SMART+ generates the lowest $\Delta STEC$ values. $\Delta STEC$ of the methods Rotation and 485 Exponential decay are in most of the cases higher than SMART+ delta STEC values and lower than the NeQuick 486 model. $\Delta STEC$ of the method Rotation with exponential decay is similar to the NeQuick model.

487 Figure 11Figure 7 and Figure 12Figure 8 present the distribution of $\Delta STEC$ and the *RMS* error (cf. Eq. (15)(14)) 488 for the quiet and perturbed periods respectively. Figure 11Figure 7 confirms the conclusions we draw so far from 489 Figure 8Figure 4 and Figure 9Figure 5. SMART+ delivers the lowest $\Delta STEC$ and *RMS* values, followed by the 490 method Rotation and then by the method Exponential decay. Rotation with exponential decay performs similar to 491 the NeQuick model. For the perturbed period, again SMART+ delivers the lowest $\Delta STEC$ and *RMS* statistics, 492 followed by the Exponential decay and the Rotation with similar results.

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493 4.3 Validation with independent space-based sTEC data

494 In order to validate the methods with respect to their capability to estimate independent STEC, the LEO satellites

- Swarm A and GRACE are chosenhave been used. The STEC measurements of these satellites are not assimilated
 by the tested methods. It is to mention here that 2015 the Swarm A satellite was flying site on site with the Swarm
- 497 C satellite at around 460 km height. The height of the GRACE orbit was around 450 km. All satellites were flying
- 498 on almost polar orbits.
- For each of the three LEOs, the residuals between $STEC^{meas}$ and $STEC^{est}$ are calculated and denoted as $dTEC = STEC^{meas} STEC^{est}$. Further, the absolute values of the residuals |dTEC| are considered.
- In general, for the quiet period, the STEC measurements of Swarm A vary below 105 TECU and for the second
 period below 170 TECU. For the GRACE satellite, the STEC measurements are below 282 TECU for the quiet
 period and below 264 TECU for the second period.
- Figure 13Figure 9 and Figure 14Figure 10 display the histograms of the STEC residuals during the quiet period
 for Swarm A and GRACE respectively. Presented are the distributions of the residuals *dTEC* and the absolute
 residuals |*dTEC*|. Also plotted are the median, STD and RMS of the corresponding residuals. Figure 15Figure
 and Figure 16Figure 12 depict the histograms of the STEC residuals during the perturbed period.
- Again, the NeQuick model seems to underestimate the measured STEC during both periods for GRACE and
- 509 Swarm A satellites. Compared to the NeQuick model, during both periods, the methods SMART+ and Exponential
- 510 decay decrease the residuals and the absolute residuals between measured and estimated STEC for both GRACE
- and Swarm A satellites. The method Rotation with exponential decay performs for both periods very similar to the
- 512 NeQuick model. The performance of the method Rotation is partly even worse than the one of the background
- 513 model. Our impression is that the number and the distribution of the assimilated measurements is too small and
- angle limited to be sufficient to dispense with a background model, as is the case with the Rotation method, which
- 515 uses the model only for the estimation of the systematic error.
- 516 Regarding the STEC of Swarm A, the lowest residuals and the most reduction in comparison to the NeQuick
- 517 model, are achieved by SMART+. The median and the STD of the SMART+ residuals are ~ 0.3 TECU and ~ 3.4
- 518 TECU resp<u>ectively</u>, for quiet and ~ 0.7 TECU and ~ 7 TECU for the perturbed period. Compared to the NeQuick
- 519 model, the absolute median value is reduced up to 64% by SMART+ during the quiet and by up to 61% during the
- 520 perturbed period. The STD value is decreased by up to 47% during the quiet and up to 29% during the storm
- 521 period. The second lowest residuals are achieved by the Exponential decay here the median of the residuals is
- around 0.2 TECU for quiet and around 0.8 TECU for the perturbed period.
- 523 Regarding the STEC of GRACE during the quiet period, the lowest residuals and the most reduction in comparison
- 524 to background, are achieved by the Exponential decay, followed by SMART+. Exponential decay reduces the
- background absolute median value by up to 26% and the STD value by up to 28%. The median of the residuals is
- around 0.2 TECU. For SMART+, the median of the residuals is around 2.9 TECU. During the perturbed period,
- 527 SMART+ reduces the absolute median at most by 17% and the STD by 9%, the Exponential decay does not reduce
- 528 the absolute median, compared to NeQuick, but it reduces the absolute STD value by 23%. The median of the
- residuals are around -0.5 TECU for Exponential decay and around 0.8 TECU for SMART+.

- 530 Comparing between quiet and storm conditions, in general an increase of RMS and STD of the SWARM A
- 531 residuals is observable for the NeQuick model and all tomography methods regarding both satellites. This is not
- 532 the case for the GRACE residuals.

533 4.4 Validation with independent LP in-situ electron densities

In this section, we further extend our analyses to the validation of the methods with independent LP in-situ electron densities of the three Swarm satellites. According to the locations of the LP measurements, the estimated electron density values are interpolated (by a 3D interpolation, using the MATLAB build-in function scatteredInterpolan.m) from the 3D electron density reconstructions. For each satellite, the measured electron density Ne^{meas} is compared to the estimated one Ne^{est} . In particular we calculate the residuals $dNe = Ne^{meas} Ne^{est}$, the absolute residuals |dNe|, the relative residuals $dNe_{rel} = \frac{dNe}{Ne^{meas}} \cdot 100\%$ and the absolute relative residuals $|dNe_{rel}|$.

- **Figure 17**Figure 13 depicts the distribution of the residuals dNe for the quiet period along with the median, STD and RMS values. Each of the three subplots presents one of the Swarm satellites. In Figure 18Figure 14 the histograms of |dNe| and $|dNe_{rel}|$ are given for the same period. In Figure 18Figure 14 we do not separate the values for the different satellites, because these are similar. Figure 19Figure 15 and Figure 20Figure 16 show the corresponding histograms for the perturbed period.
- The electron densities of the NeQuick model are in median slightly higher than the LP in-situ measurements for all three satellites during both periods. The median and STD values for the $|dNe_{rel}|$ residuals produced by NeQuick are ~33% and ~38% resp. during the quiet period. For the perturbed period, we observe higher median and STD values of ~45% and ~56%, resp. The increase of the RMS and STD values of the absolute residuals is also visible for all the considered reconstruction methods.
- 551 The methods SMART+ and Rotation with exponential decay follow the trend of the model and show similar 552 distributions in Figure 17Figure 13 and Figure 19Figure 15. Comparing these two methods with the NeQuick 553 model, the performance of SMART+ is slightly better reducing the median of the absolute and absolute relative 554 residuals by up to 8%. Further, during both periods, SMART+ reduces the STD values of the |dNe| values by up 555 to 23%. However, the STD and RMS values of the $|dNe_{rel}|$ residuals for SMART+ during the quiet period are higher than those of the NeQuick model. The median and STD values of the $|dNe_{rel}|$ residuals for SMART+ are 556 557 \sim 30% and \sim 43% resp. during quiet and higher during perturbed period, namely \sim 43% and \sim 53% resp. The 558 statistics of the methods Exponential decay and Rotation are worse than those of NeQuick.
- 559

560 5 Summary and conclusions

In this paper, we focus on the assessment of assess three different propagation methods for an Ensemble Kalman Filter approach in the case that a physical propagation model is not available or discarded due to computational burden. We validate these methods with independent STEC observations of the satellites GRACE and Swarm A and with independent Langmuir probes data of the three Swarm satellites. The methods are compared to the algebraic reconstruction method SMART+, serving as a benchmark and to the background model NeQuick-model for periods of the year 2015 covering quiet to perturbed ionospheric conditions. This work is carrying out our first
 case study in this regard.

568 Overlooking all the validation results, the methods SMART+ and Exponential decay reveal the best performance 569 with the lowest residuals. In general,, whereas the method Rotation with exponential decay provides only a small 570 improvement compared to the -NeQuick model. While SMART+ modifies the electron densities of the background 571 model around the measurement geometry and produces rather small patches, the EnKF produces larger and are 572 smoother patterns. As expected, the validations indicate that the electron density estimates of the EnKF are not 573 only dependent on the current measurement geometry but also on prior assimilations.

574 In summary, the comparison with the assimilated The plausibility check in section 4.2 STEC shows that during

- 575 both periods all methods reduce successfully the median, RMS and STD values of the STEC residuals and provide
- 576 better results in comparison to than the background model. SMART+ demonstrates the best performances at best

577 <u>improving</u>and lowers the errorthe statistics of the NeQuick model by up to 86%, followed by the method Rotation,

578 decreasing the median of the residuals by up to 83%. The method Exponential decay lowers reduces the median

579 by up to 55%, but the STD values stay almost on the same level as for the NeQuick model.

580 Although the EnKF with the method Rotation reproduces the assimilated STEC data well, less accurate estimates

581 are obtained in the validation with independent data. We assume this has two main reasons: First, as the only

582 propagation method, Rotation is not anchored by the background model. Second, the number of the assimilated

- 583 measurements is low compared to the number of unknowns and the available measurements are unevenly
- 584 distributed and angle limited. Both together could lead to increased deviations of the estimates from the truth.
- 585

Regarding the ability to estimate independent STEC measurements, <u>T</u>the methods SMART+ and <u>the EnKF with</u>
Exponential decay <u>provide the best estimates of the independent STEC and</u> reduce the <u>independent</u> STEC residuals
by up to 64% for Swarm A and 28% for GRACE, compared to the NeQuick model. SMART+ generates the
smallest residuals for the STEC measurements of Swarm A and Exponential decay performs at best for STEC
measurements of GRACE.

591 Concerning the estimation of independent electron densities of the <u>yLangmuir Probes-data</u>, SMART+ shows the 592 best results, reducing the background statistics of the absolute residuals by up to 23%. The median and STD values 593 of the absolute residuals $|dNe_{rel}|$ for SMART+ are ~30% and ~43% respectively- during quiet ionospheric 594 conditions and higher, namely ~43% and ~53% respectively- during perturbed ionospheric conditionsperiod. The 595 distributions of the residuals produced by Rotation with exponential decay are similar to the ones of the NeQuick 596 model. In general, all the considered methods generate relatively high residuals.

These observations could be explained by the fact-It should be noted here that the independent electron density measurements are located at the lower edge of the reconstructed area and all the assimilated measurements are located above. Additionally, <u>as already mentioned in Section 3.3.2</u>, Swarm LPs was found to underestimate the true electron density systematically, <u>cf. Section 3.3.2</u>. In order to <u>This could be the second reason</u>, why the reconstructions, based on the STEC, do not match the LPs electron densities. To get <u>obtain</u> better results for the lower altitudes, it might <u>therefore</u> be necessary to apply a kind of anchor point from below<u>for the lower altitudes</u> within the reconstruction procedure. We plan to utilise which could for instance be therefore the Swarm LPs

604 electron den<u>si</u>isty measurements themselves.

- Another approach to improve the reconstructions could be to precondition the background model, e.g. in terms of
- F2 layer characteristics or the plasmapause location (cf. e.g. Bidaine and Warnant, 2010, Gerzen et. al., 2017).

- 608 <u>TFurther, to get a comprehensive final concluding</u> impression of the performance of the investigated methods and
- to $\frac{1}{\text{get angain}}$ insight into the ability of the methods $\frac{1}{\text{tofor}}$ correctly characterize the shapes of the electron
- 610 density profile-shapes, we intend to continue the validation of the methods with additional independent
- 611 measurements of the plasmasphere and topside ionosphere, e.g. coherent scatter radar data, and plasmasphere.
- 612 start to work on comparisons with independent electron density data, located in the plasmasphere and with
- 613 coherent scatter radar data.
- 614 Furthermore, a pre-adjustment of the background model, e.g. in terms of F2 layer characteristics or the
- 615 plasmapause location, may be helpful to improve the reconstruction results (cf. e.g. Bidaine and Warnant, 2010,
- 616 Gerzen et. al., 2017).

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627 References

- Angling, M. J.: First assimilation of COSMIC radio occultation data into the Electron Density Assimilative Model
 (EDAM), Ann. Geophys., 26, 353-359, 2008.
- Angling, M. J. and Cannon, P. S.: Assimilation of radio occultation measurements into background ionospheric
 models, Radio Sci., 39, RS1S08, doi:10.1029/2002RS002819, 2004.
- 632 Banville, S.: Improved convergence for GNSS precise point positioning. Ph.D. dissertation, Department of
- 633 Geodesy and Geomatics Engineering, Technical Report No. 294, University of New Brunswick, Fredericton, New
- 634 Brunswick, Canada, 2014.
- Bidaine B. and R. Warnant: Assessment of the NeQuick model at mid-latitudes using GNSS TEC and ionosonde
- 636 data, Adv. Space Res., 45, 1122-1128, 2010.
- Bilitza, D., L.-A. McKinnell, B. Reinisch, and T. Fuller-Rowell: The International Reference Ionosphere (IRI)
 today and in the future, J. Geodesy, 85:909-920, DOI 10.1007/s00190-010-0427-x, 2011.
- Bust, G. S., and C. N. Mitchell: History, current state, and future directions of ionospheric imaging, Rev. Geophys.,
 46, RG1003, doi:10.1029/2006RG000212, 2008.
- 641 Chen P., Y. Yao: Research on global plasmaspheric electron content by using LEO occultation and GPS data, Adv.
 642 Space Res., 55, 2248–2255, doi:10.1016/j.asr.2015.02.004, 2015.
- 643 Codrescu, S. M., M. V. Codrescu, M. Fedrizzi: An Ensemble Kalman Filter for the thermosphere-ionosphere.Space
- 644 Weather, 16, 57–68, https://doi.org/10.1002/2017SW001752, 2018.
- 645 Dettmering D.: Die Nutzung des GPS zur dreidimensionalen Ionosphärenmodellierung. PhD Thesis, University of
- 646 Stuttgart, http://elib.uni-stuttgart.de/opus/volltexte/2003/1411/, 2003.

- Elvidge, S., and M. J. Angling: Using the local ensemble Transform Kalman Filter for upper atmospheric
 modelling, J. Space Weather Space Clim., 9, A3, https://doi.org/10.1051/swsc/2019018, 2019.
- Evensen, G.: Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte Carlo methods
 to forecast error statistics, J. Geophys. Res., 99 (C5), 10143–10162, doi:10.1029/94JC00572, 1994.
- Evensen, G.: The Ensemble Kalman Filter: theoretical formulationand practical implementation, Ocean Dynamics,
 53, 343-367, DOI 10.1007/s10236-003-0036-9, 2003.
- Howe, B. M., K Runciman, J. A. Secan, Tomography of the ionosphere: Four-dimensional simulations, Radio Sci.,
 33, 1, 109-128, 1998.
- Gerzen, T., Minkwitz, D., and Schlueter, S.: Comparing different assimilation techniques for the ionospheric F2
 layer reconstruction, J. Geophys. Res.-Space, 120, 6901–6913, doi:10.1002/2015JA021067, 2015.
- Gerzen, T. and D. Minkwitz, Simultaneous multiplicative column normalized method (SMART) for the 3D ionosphere tomography in comparison with other algebraic methods, Ann. Geophys., 34, 97-115, doi: 10.5194/angeo-34-97-2016, 2016.
- Gerzen, T., V. Wilken, D. Minkwitz, M. Hoque, S. Schlüter: Three-dimensional data assimilation for ionospheric
 reference scenarios, Ann. Geophys., 35, 203-215, doi:10.5194/angeo-35-203-2017, 2017.
- Heise, S., N. Jakowski, A. Wehrenpfennig, Ch. Reigber, H. Lühr: Sounding of the topside
 ionosphere/plasmasphere based on GPS measurements from CHAMP: Initial results, Geophys. Res. Letters,
 29(14), doi: 10.1029/2002GL014738, 2002.
- Hernandez-Pajares, M., J.M. Juan, J. Sanz: New approaches in global ionospheric determination using ground
 GPS data. J Atmos Solar Terr Phys, 61: 1237-1247, 1999.
- Hochegger G., Nava B., Radicella S.M., and R. Leitinger: A Family of Ionospheric Models for Different Uses,
 Phys. Chem. Earth Part C Solar Terres Planet Sci, 25, 307-310, doi:10.1016/S1464-1917(00)00022-2, 2000.
- Howe B., K. Runciman: Tomography of the ionosphere: Four-dimensional simulations, Radio Sci., 33, 1, 09-128,1998.
- Kalnay, E.: Atmospheric Modeling, Data Assimilation and Predictability, Cambridge University Press,
 Cambridge, UK, 2011.
- Klimenko M. V., V. V. Klimenko, I. E. Zakharenkova, I. V. Cherniak: The global morphology of the
 plasmaspheric electron content during Northern winter 2009 based on GPS/COSMIC observation and GSM TIP
 model results. Adv. Space Res., 55, 2077–2085, doi:10.1016/j.asr.2014.06.027, 2015
- Lee, I. T., T. Matsuo, A. D. Richmond, J. Y. Liu, W. Wang, C. H. Lin, J. L. Anderson, M. Q. Chen: Assimilation of FORMOSAT-3/COSMIC electron density profiles into a coupled thermosphere/ionosphere model using ensemble Kalman filtering, JGR, 117, A10, https://doi.org/10.1029/2012JA017700, 2012.
- Liang, W., M. Limberger, M. Schmidt, D. Dettmering, U. Hugentobler, D. Bilitza, N. Jakowski, M.M. Hoque, V.
 Wilken, T. Gerzen: Regional modeling of ionospheric peak parameters using GNSS data an update for IRI. Adv.
- 681 Space Res., 55(8), 1981-1993, 10.1016/j.asr.2014.12.006, 2015.
- 682 Liang, W., M. Limberger, M. Schmidt, D. Dettmering, U. Hugentobler: Combination of ground- and space-based
- 683 GPS data for the determination of a multi-scale regional 4-D ionosphere model. In: Rizos C., Willis P. (Eds.) IAG
 684 150 Years, IAG Symposia, 143, 751-758, 10.1007/1345_2015_25, 2016.
- 685 Lomidze, L., L. Scherliess, R. W. Schunk: Magnetic meridional winds in the thermosphere obtained from Global
- Assimilation of Ionospheric Measurements (GAIM) model, JGR: Space Physics, 120, 9, 8025-8044, https://doi.org/10.1002/2015JA021098, 2015.
- Lomidze, L., D. J. Knudsen, J. Burchill, A. Kouznetsov, S. C. Buchert: Calibration and validation of Swarm plasma
 densities and electron temperatures using ground-based radars and satellite radio occultation measurements, Radio
 Sci., 53, 15–36, https://doi.org/10.1002/2017RS006415, 2018.
- Minkwitz, D., K.G. van den Boogaart, T. Gerzen, M.M. Hoque: Tomography of the ionospheric electron density
 with geostatistical inversion, Ann. Geophys., 33, 1071–1079, https://doi.org/10.5194/angeo-33-1071-2015, 2015.
- Minkwitz, D., K. G. van den Boogaart, T. Gerzen, M. Hoque, M. Hernández-Pajares: Ionospheric tomography by
 gradient enhanced kriging with STEC measurements and ionosonde characteristics, Ann. Geophys., 34, 999-1010,
 doi:10.5194/angeo-34-999-2016, 2016.
- Nava B., P. Coisson, and S.M. Radicella: A new version of the NeQuick ionosphere electron density model, J.
 Atmos. Sol-Terr. Phy., 70, 1856-1862, doi:10.1016/j.jastp.2008.01.015, 2008.
- Nikoukar, R., G. Bust, D. Murr: Anovel data assimilation technique for the plasmasphere, J. Geophhys. Res.,
 Space Physics, 120, 8470-8485, doi:10.1002/2015JA021455, 2015.
- Odijk, D.: Precise GPS positioning in the presence of ionospheric delays. Publications on geodesy, Vol. 52. The
 Netherlands Geodetic Commission, Delft. ISBN-13: 978 90 6132 278 8, 2002.

- 702 Olivares-Pulido G., M. Terkildsen, K. Arsov, P.J.G. Teunissen, A. Khodabandeh, V. Janssen: A 4D tomographic
- 703 ionospheric model to support PPP-RTK, Journal of Geodesy, 93, 9, 1673-1683, https://doi.org/10.1007/s00190-704 019-01276-4, 2019.
- 705 Radicella S. M., and R. Leitinger: The evolution of the DGR approach to model electron density profiles, Adv. 706 Space. Res., 27, 35-40, doi:10.1016/S0273-1177(00)00138-1, 2001.
- 707 Schaer, S.: Mapping and predicting the Earth's ionosphere using the global positioning system. Ph.D. dissertation, 708 Astron Institute, University of Bern, Berne, 1999.
- 709 Scherliess, L., D. C. Thompson, R. W. Schunk: Ionospheric dynamics and drivers obtained from a physicsbased 710 data assimilation model, Radio Sci., 44, RS0A32, doi:10.1029/2008RS004068, 2009.
- 711 Schmidt, M., D. Bilitza, C. Shum, C. Zeilhofer: Regional 4-D modelling of the ionospheric electron density. Adv Space Res 42: 782790. https://doi.org/10.1016/j.asr.2007.02.050, 2008. 712
- 713 Schmidt, M., D. Dettmering, F. Seitz: Using B-spline expansions for ionosphere modeling. In: Freeden W., Nashed
- 714 M.Z., Sonar T. (Eds.) Handbook of Geomathematics (Second Edition), 939-983, Springer, 10.1007/978-3-642-715 54551-1 80, 2015.
- 716 Schunk, R. W., et al.: Global Assimilation of Ionospheric Measurements (GAIM), Radio Sci., 39, RS1S02, 717 doi:10.1029/2002RS002794, 2004.
- 718 Schunk, R. W., L. Scherliess, V. Eccles, L. C. Gardner, J. J. Sojka, L. Zhu, X. Pi, A. J. Mannucci, M. Butala, B.
- 719 D. Wilson, A. Komjathy, C. Wang, G. Rosen: Space weather forecasting with a Multimodel Ensemble Prediction System (MEPS), Radio Sci., 51, 1157-1165, doi:10.1002/2015RS005888, 2016. 720
- 721 Spencer, P. S. J., C. N. Mitchell: Imaging of 3-D plasmaspheric electron density using GPS to LEO satellite differential phase observations, Radio Sci., 46, RS0D04, https://doi.org/10.1029/2010RS004565, 2011. 722
- 723 Wang, C., G. Hajj, X. Pi, I. G. Rosen, B. Wilson: Development of the Global Assimilative Ionospheric Model, 724 Radio Sci., 39, RS1S06, doi:10.1029/2002RS002854, 2004.
- 725
- Wen, D., Y. Yuan, J. Ou, X. Huo, K. Zhang: Three-dimensional ionospheric tomography by an improved algebraic 726 reconstruction technique, GPS Solut., 11, 251-258, doi:10.1007/s10291-007-0055-y, 2007.
- 727 Wen, D., D. Mei, Y. Du: Adaptive Smoothness Constraint Ionospheric Tomography Algorithm, Sensors (Basel), 728 20, 8, doi: 10.3390/s20082404, 2020.
- 729 Zeilhofer, C.: Multi-dimensional B-spline Modeling of Spatio-temporal Ionospheric Signals: DGK. Series A, 123,
- 730 München, 2008.
- 731 Zeilhofer, C., M. Schmidt, D. Bilitza, C. K. Shum: Regional 4-D modeling of the ionospheric electron density
- 732 from satellite data and IRI, Adv. Space Res., 43, 2009.
- 733



735 Figure 1: The distribution of the ensemble residuals for a chosen altitude and selected UT times, for all

736 latitudes, longitudes. Left-:- for DOY 041, right-: -- for DOOY 076.



739 Figure 2: Subfigures top: Rotation with exponential decay reconstructed electron density represented by

layers at different heights between 490 and 827 km (left) and at chosen longitudes for altitudes between 827
 and 2400 km (right). Subfigures bottom: The vertical TEC map deduced from the reconstructed (left) and

742 NeQuick-modeled (right) 3D electron density in the altitude range between 450 and 20200 km.



Figure 3: Subfigures top: Method Rotation reconstructed electron density represented by layers at different
heights between 490 and 827 km (left) and vertical TEC map deduced from the reconstructed 3D electron
density in the altitude range between 450 and 20200 km (right).





Figure 5: Differences between reconstructed and NeQuick modeled electron density <u>in percent</u>, represented
 by layers at different heights between 490 and 827 km. Left top: For Rotation with exponential decay. Right
 top: <u>Method</u> Rotation. Left bottom: <u>Method</u> Exponential decay. Right bottom: SMART+.



Figure 6: The locations of the LEO satellites <u>offor</u> the STEC measurements used for the reconstruction.



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exponential decay. Middle: Rotation. Bottom: Exponential decay.



Figure <u>84</u>: Plausibility check – distributions of the STEC measured <u>minus</u>– STEC estimated residuals. Left
 subfigure depicts residuals of the quiet period, right subfigure for the perturbed period.



6

Delta STEC / TECU



0 ' 0

3

775 Figure 117: Plausibility check for the quiet period – distributions of the delta TEC (left) and RMS (right) 776 values.

0.0

6

9 RMS STEC / TECU

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Rot and Exp

Rot

Exp NeQuick

-SMART+



(right) values.



Figure <u>13</u>9: Histograms of the STEC residuals (left) and absolute residuals (right) during the quiet period, for Swarm A.







Figure <u>15</u>11: Histograms of the STEC residuals (left) and absolute residuals (right) during the perturbed

788 period, for Swarm A.



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Figure <u>1612</u>: Histograms of the STEC residuals (left) and absolute residuals (right) during the perturbed period, for GRACE.















Figure 1915: Validation with LP data – distribution of the Swarm A, B, C (separated) electron density residuals for the perturbed period.



Figure 2016: Validation with LP data – distribution of the Swarm absolute and absolute relative electron density residuals for the perturbed period.